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# COMPUTER PROGRAM FOR CALCULATION OF A GAS TEMPERATURE PROFILE BY INFRARED EMISSION - ABSORPTION SPECTROSCOPY

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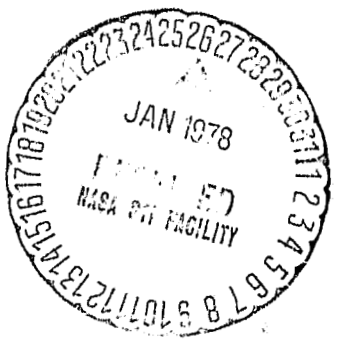

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16. Abstract

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CONTENTS

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## SUMMARY

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## INTRODUCTION

Infrared emission and absorption measurements at two or more wavelengths provide a means of determining a gas temperature profile along a path through the gas by using a radiation source and receiver located only at the ends of the path (ref. 1). In the case of a jet engine or rocket engine exhaust stream, the instrumentation may be outside of the stream. The method has been termed the "spectral-scanning method." Practical instruments that permit use of this technique are described in references 1 through 4.

Tests of the method with heated pure gases in a furnace of 60 cm path length (ref. 2), and then with flames over a 22 cm path length

(ref. 3) gave good results. An analysis in reference 5 showed the effect of radiometric errors on the accuracy of the computed profile. The analysis assumed the partial pressure of the radiating gas was a constant over the entire path, with the constant determined from radiometric measurements. More recently, the feasibility of using only emission measurements and an estimated gas composition to determine industrial furnace temperature profiles over a 10-meter path length at atmospheric pressure has been shown (ref. 6).

The computer program presented herein involves an iterative, cyclic computation in which an initial assumed (arbitrary but realistic) temperature profile is altered in shape until the computed emission and absorption that it would yield agree as closely as possible with the actual instrumental measurements of emission and absorption. The procedure requires the use of a large-scale computer. These procedures have been outlined in principle in previous publications; but this report presents an actual program that has been found to produce useful results.

The present work also extends the work of reference 5 by providing greater latitude in the temperature-profile shape that can be treated and by relaxing restrictions on the shape of the associated pressure profile. Thus, whereas previous studies have principally treated profiles with a substantial temperature difference over the optical path, the present study also includes the equally important case of an almost isothermal profile; and whereas the work of reference 5 has assumed constant pressure over the path, the present work allows an additional degree of freedom in the description of the pressure profile.

The program presented provides a means of determining temperature from experimental measurements of emission and absorption at two or more wavelengths. But it also provides a means, before any experiments are performed, of selecting those wavelengths whose use will lead to the best attainable accuracy. This prior selection is very important, because a poor selection of wavelengths may lead to unacceptably high uncertainty in the temperature and may even lead to an erroneous solution of the equations. The existence and avoidance of this incorrect solution for the

temperature profile is demonstrated. Thus, this report provides the potential user with a means of determining whether this method will be sufficiently accurate for his particular application, as well as providing a means of finding the solution if the method is adopted. Symbols are listed in appendix A.

## MATHEMATICAL ANALYSIS

### Method of Determining Temperature and Pressure Profiles

The method is iterative with each iterative step consisting of three principal parts:

1. With current profiles of temperature and pressure, compute the gas radiance and transmittance at each wavelength of measurement.

2. Record the difference between computed and measured gas radiance and transmittance at each wavelength of measurement.

3. Correct the current profiles in (1) to reduce the differences in (2) to zero.

Functional forms of the temperature profile $T(x)$ and the partial pressure profile $p(x)$ of the absorbing gas are assumed in advance. The temperature profile is expressed in terms of two unknown parameters, and the pressure profile in terms of one unknown parameter. A minimum of one set of measurements, at each of two wavelengths, is required to yield a solution for the unknown parameters; each set actually involves four radiometric measurements (i.e., four instrument readings). The computational program then determines, from the simultaneous solution of equations containing actual radiometric measurements, the values of these parameters that make computed values of radiance and transmittance equal to measured values.

Additional wavelengths of measurement may improve accuracy, in such case, a least-squares method of solution is employed. The results obtained are the values of the parameters when the "residual", which is the sum of the squares of the differences between measured and computed values of radiance, is a minimum.

The functions used in this program may be modified as desired for a particular application. However, tests during development of the program have shown that it is impractical to characterize the temperature profile by more than two unknown parameters because the accuracy of the solution becomes unacceptably low.

The profiles. - In the present program, the profiles are taken to be axisymmetric, with shapes chosen to resemble the transverse pressure and temperature distributions often found in ducts. The functions are expressed in terms of values of the dependent variable at the axial, or centerline, position (subscript c) and at a wall position (subscript w), and the value of a shape parameter $\eta_T$ or $\eta_p$ for temperature or pressure, respectively.

1. When the temperature profile is far from isothermal, it is taken as

$$T(x) = T_c - (T_c - T_w)|y|^{1/\eta_T} \tag{1}$$

where

$$y = (2x/L) - 1 \qquad 0 \le x \le L$$

It is assumed that $T_w$ is measured independently. Parameters $T_c$ and $\eta_T$ are determined by the computational program. They are then termed the dependent parameters. This family of curves is shown in figure 1(a).

2. When the profile is nearly isothermal, except for a thin boundary layer at each end, the temperature profile is taken as

$$T(x) = T_c - (T_c - T_w^*)|y|^{1/\eta_T} \tag{2a}$$

where

$$y = (2x/L) - 1 \qquad x_1 \le x \le L - x_1$$

and

$$T(x) = T_w + (T_1 - T_w)z + (mx_1 + T_w - T_1)z(z - 1) \qquad 0 \le z \le 1 \qquad (2b)$$

where

$$z = x/x_1 \qquad \text{for} \quad 0 \le x \le x_1$$

$$z = (L - x)/x_1 \qquad \text{for} \quad L - x_1 \le x \le L$$

$$T_1 = T(x_1) = T(L - x_1)$$

$$m = (dT/dx)_{x=x_1} = 2(T_c - T_1)/\left[\eta_T(L - 2x_1)\right]$$

This definition of $T(x)$ provides continuity of both temperature and temperature gradient at $x = x_1$ and at $x = L - x_1$. This family of curves is shown in figure 1(b). Using this definition, $\eta_T$ and $x_1$ are preassigned some reasonable values and the computational program determines $T_w^*$ and $T_c$ as the dependent parameters. It is assumed that $T_w$ is measured independently.

3. The partial pressure profile of each absorbing gas is assumed to be of the form

$$p(x) = p_c - (p_c - p_w)|y|^{1/\eta_p} \qquad (3)$$

where

$$y = (2x/L) - 1 \qquad 0 \le x \le L$$

The profile is shown in figure 1(c). Different initial values may be assumed for parameters $p_c$, $p_w$, and $\eta_p$ for each gas. The choice of th initial values of the parameters may be aided by a computation of the partial pressure of the reaction products. These pressures can be computed for a range of reaction product temperatures and a range of partial pressures

and reactant composition using the computer program of reference 7. From these data a choice for initial values of the pressure parameters can be made. (The program of ref. 7 may be obtained from its authors, on written request, by sending a magnetic tape at least 1200 ft long and by specifying the type of computer. Parts of the program not used in this application may be removed after the program has been transferred from tape to cards.)

Tests during the development of the program for computing temperature and pressure profiles have shown that only one dependent pressure parameter can be determined with acceptable accuracy. This is best done by designating the parameter $p_{c,1}$ of the principal absorbing gas (subscript 1) as an independent parameter. The wall pressure $p_{w,1}$ is selected to be directly proportional to the center pressure, and the shape parameter $n_{p,1}$ is chosen judiciously and held constant. Assumed parameters for all other absorbing gases (subscript k) and all nonabsorbing gases (subscript j) determine the initial pressure profiles $[p_k(x)]_o$ and $[p_j(x)]_o$.

Next, these profiles are made dependent on the profile $p_1(x)$. The absorbing gases initially have profiles that determine ratios $[p_k(x)/p_1(x)]_o$. Then, as $p_1(x)$ is changed by the program, these other profiles are also changed by the linear relation

$$p_1(x)[p_k(x)/p_1(x)]_o \tag{4}$$

After the absorbing-gas pressure profiles are determined, the nonabsorbing-gas pressure profiles $p_j(x)$ are adjusted to make the sum of all gas pressures equal to the measured static pressure $p_S$ which is assumed to be independent of x, so that

$$p_S = \sum_k p_k(x) + \sum_j p_j(x)$$

An additional constraint is to maintain the relative amounts of each nonabsorbing gas as given by the initial profiles, that is, in the ratio

$$\left[p_j(x)/\sum_j p_j(x)\right]_o$$

Thus the pressures of the nonabsorbing gases are given by

$$p_j(x) = \left[p_s - \sum_k p_k(x)\right]\left[p_j(x)/\sum_j p_j(x)\right]_o \tag{5}$$

The residuals. - Initial values of all parameters of the profile functions are tabulated, and the resultant sets of values of gas radiance $N_L$ and transmittance $\tau_L$ are computed for two or more wavelengths from radiometric equations. The computed quantities are denoted by ${}^cN_L$ and ${}^c\tau_L$. The corresponding measured quantities at the same wavelengths are denoted by ${}^mN_L$ and ${}^m\tau_L$. The difference between the computed and measured quantities is called the "residual." The residual for gas radiance may be expressed as a fractional value

$$R_N = ({}^cN_L - {}^mN_L)/{}^mN_L \tag{6}$$

It is preferable to use gas absorptance $\alpha_L = 1 - \tau_L$ in place of transmittance $\tau_L$ for the transmittance residual because $\alpha_L$ is more nearly proportional to the gas pressure and to the gas absorption coefficient. The residual for gas absorptance is defined as

$$R_\alpha = ({}^c\alpha_L - {}^m\alpha_L)/{}^m\alpha_L = ({}^m\tau_L - {}^c\tau_L)/(1 - {}^m\tau_L) \tag{7}$$

The solution. - The solution is reached by reducing the residuals to an acceptably small value by appropriately changing the two variable parameters in the equation for the temperature profile and the one variable parameter in the equation for the pressure profile. This is done iteratively using the Newton-Raphson method (ref. 8, p. 175) because the equations are nonlinear. For two wavelengths of measurement each

iterative step involves the solution of the following three simultaneous equations for the increments $\Delta y_j$ to the current value of the three variable parameters represented by $y_j$,

$$\left.\begin{aligned}
(1)\sum_j \left(\frac{1}{m_{N_{\lambda_1},L}} \cdot \frac{\partial^c N_{\lambda_1},L}{\partial y_j}\right)\Delta y_j &= -R_{\lambda_1,N} \\
(2)\sum_j \left(\frac{1}{m_{N_{\lambda_2},L}} \cdot \frac{\partial^c N_{\lambda_2},L}{\partial y_j}\right)\Delta y_j &= -R_{\lambda_2,N} \\
(3)\sum_j \left(\frac{1}{m_{\alpha_{\lambda_1},L}} \cdot \frac{\partial^c \alpha_{\lambda_1},L}{\partial y_j}\right)\Delta y_j &= -R_{\lambda_1,\alpha}
\end{aligned}\right\} \qquad (8)$$

Note that only one wavelength is needed for $R_{\lambda_1,\alpha}$ to determine one pressure parameter. The derivatives in equation (8) are obtained numerically. The final value of the residuals is zero.

There are cases where there are more measurements than there are variable parameters. For these cases, where the final values of the residuals are not necessarily zero, a damped least-squares modification of equation (8) is used to find a solution at which

$$R^2_{\lambda_1,\alpha} + \sum_i R^2_{\lambda_i,N} \equiv R^2 = \text{a minimum} \qquad (9)$$

where there are as many residuals $R_N$ as there are i wavelengths, and there is only one residual $R_\alpha$. The damped least squares method is used in this program. Its derivation is in the second part of appendix B.

In addition to the solution for the profile parameters, an estimate is made of the error in the parameters that would be caused by stated random errors of radiometric measurements and tabulated absorption coefficients. (Typical orders of magnitude for these errors are 1 percent in radiation and 5 percent in absorption coefficient.) The error equation is derived in appendix B.

## Measurement of Gas Radiance and Transmittance

The actual gas radiance $N_L$ and transmittance $\tau_L$ are derived from measurements of detector (radiometer) output voltage $V$ that is assumed to be proportional to incoming radiant power. The factor of proportionality (calibration factor) of the detector includes the effect of all optics between the radiometer element and the gas, but it need not be known explicity if it remains constant for all measurements. The optics include, in addition to windows, lenses, and stops, a monochromator of bandwidth $\Delta\lambda$ centered on wavelength $\lambda$. The following measurements of detector output voltage $V$ are made:

(a) $V_o$, where a calibrated source of radiance $N_o$ is placed at the gas location, in place of the gas.

(b) $V_1$, due to radiation from the gas.

(c) $V_2$, where a stable comparison source radiates through the gas path, but the gas is absent.

(d) $V_3$, when the comparison source radiates through the gas path in the presence of the gas.

By chopping the radiation from the comparison source at a unique, distinctive frequency, voltages $V_1$ and $V_3$ are distinguished from each other, and voltage $V_3$ does not include gas radiation (ref. 1, p. 28).

These four measurements yield

$$N_L = N_o \frac{V_1}{V_0}; \quad \tau_L = \frac{V_3}{V_2} \tag{10}$$

## Computation of Gas Radiance and Transmittance

The gas radiance, integrated over a narrow wavelength band $\Delta\lambda$ centered at $\lambda$ and over a path length $L$, is

$$N_L = \int_0^L N_\lambda^* \left(\frac{d\tau}{dx}\right) dx \tag{11}$$

where $N_\lambda^*$ is the Planck radiation function

$$N_\lambda^* = \frac{c_1}{\lambda^5} (e^{c_2/\lambda T} - 1)^{-1}$$

and $\tau$ is the gas transmittance over the path from 0 to $x$. The detailed justification for equation (11) is presented in reference 5.

The gas transmittance for a band $\Delta\lambda$ is described by a band-model formulation for a nonisothermal gas based on equation (5) of reference 9. This formulation has been justified and applied in reference 2, and summarized in reference 10. For profiles with a large variation in temperature, the formulation as modified in references 3 and 11 is adopted. Other band-models can be found in the literature (ref. 12).

The transmittance $\tau$ for a single gas is a function of the dimensionless optical depth $u$ and is given by

$$\tau = \exp\left\{\frac{-u\beta_e}{\left[1 + \left(\frac{\pi u}{2}\right)\right]^{1/2}}\right\} \tag{12}$$

For a mixture of $q$ absorbing gases the combined transmittance is the product

$$\tau = \prod_{l=1}^{q} \tau_l \tag{13}$$

The optical depth of a path length x is

$$u = \frac{1}{\beta_e} \int_0^x k \left( \frac{\beta}{\beta_e} \right)^{\eta} dx \tag{14}$$

where k is the absorption coefficient at local temperature T and partial pressure p of the absorbing gas and $\eta$ is an interpolation parameter. The parameter $\beta$ is the local value of the line overlap parameter and is given by $\beta = 2\pi\gamma/d$ where $\gamma$ is the average line width, and d is the average line spacing. The definitions of u and $\tau$ given here differ slightly in form from those of references 3 and 11 for reasons of computational expediency.

A modification in references 3 and 11 replaces the constant average $\beta_e$ of reference 2 ($\beta_{av}$ of ref. 4) by a cumulative average produced by weighting $\beta(x)$ with the absorption coefficient, so that

$$\beta_e(x) = \frac{\int_0^x k\beta \, dx}{\int_0^x k \, dx} \tag{15}$$

The interpolation parameter $\eta$ is given by one of two formulas

$$\left.\begin{aligned} \eta &= \frac{u + A_1}{u + A_2} \qquad u > A_5 \\ \eta &= \frac{uA_3}{A_5 + uA_4} \qquad u \le A_5 \end{aligned}\right\} \tag{16}$$

where

$$A_5 = 1 + 0.185 \, (\beta/\beta_e) \tag{17}$$

Values for $A_1$, $A_2$, $A_3$, $A_4$, and $A_5$ are listed in table I in terms of $(\beta/\beta_e)$.

The computation for the initially assumed profiles T(x) and p(x) first determines all values of k, $\beta$, and $\beta_e$, as functions of x from the band model data and equation (15). For example, tabulations of $k_s$ and $(\gamma/d)_s$ for $H_2O$, $CO_2$, and CO may be obtained from reference 13 or, for $H_2O$, from references 14 and 15. (The subscript s here denotes the value at standard temperature and pressure.) Values of $k_s$ in the tables are denormalized to the local gas temperature and partial pressure by

$$k = k_s p \frac{273}{T} \tag{18}$$

where p is in atmospheres and T is in kelvin. Similarly, the tabulated values of $(\gamma/d)_s = \beta_s/(2\pi)$ may be used to obtain the local value as it is affected by the line-broadening effect of all gas components in accordance with the formula

$$\beta = \beta_s\left(\sum_k \alpha_k^* p_k + \sum_j \alpha_j^* p_j\right) \tag{19}$$

where $p_j$, $p_k$ are the partial pressures, and $\alpha_j^*$, $\alpha_k^*$ are the broadening coefficients for the k absorbing gases and j nonabsorbing gases. For the absorbing gas, values of $\alpha^*$ are given in reference 16 and are listed in table II.

The path length $0 \le x \le L$ is divided into increments $\Delta x_i = x_i - x_{i-1}$ $(i = 2, \ldots)$ and the values of k, $\beta/\beta_e$, $\beta_e$ are determined at each station. Then, starting with the values $\eta_1 = 0$, $u_1 = 0$, and $\tau_1 = 1$ at $x = 0$, the following sequence of computations is made for each successive increment of path:

(1) Find $u_i = u_{i-1} + \Delta u_1$ with equation (14), using $k_i$, $(\beta/\beta_e)_1$, $(\beta_e)_i$, and $\eta_{i-1}$.

(2) Find $\eta_i$ with equations (10) and (11), using $u_i$. Linear interpolation in table I is used to find $A_1$ to $A_4$, since the computation is relatively insensitive to these quantities. Equation (11) is used to find $A_5$.

(3) Find $\tau_i$ with equation (12) using $u_i$ and $(\beta_e)_i$.

For the numerical computation, equations (14) and (15) are written

$$u_i = \frac{1}{(\beta_e)_i} \sum_{l=2}^{i} k_l \left(\frac{\beta}{\beta_e}\right)_l^{\eta_{l-1}} \Delta x_l \tag{14a}$$

$$(\beta_e)_i = \frac{\sum_{l=2}^{i} k_l \left(\frac{\beta}{\beta_e}\right)_l^{\eta_{l-1}} \Delta x_l}{\sum_{l=2}^{i} k_l \, \Delta x_l} \tag{15a}$$

## Accuracy of the Solution

There are several sources of error that affect the accuracy of the solution. First there is the basic limitation of the functional forms assumed for the temperature and pressure profiles. Obviously not all situations encountered in practice can be accommodated by these functions with acceptable accuracy. For those cases other functional forms must be used. This basic limitation is demonstrated in the section "Application of the Program to an Experiment" where an example is worked out for a temperature profile that cannot be matched exactly by the assumed functional form for the temperature.

Another source of error is generated by the nature of the set of iteration equations for the parameters, equation (8). On the left side,

the matrix of derivatives may be poorly conditioned. The conditioning of the matrix is affected by the selection of the wavelengths of measurement. Proper selection of the wavelengths is treated in the next section.

The residuals on the right side of equation (8) are not exact quantities due to errors in their components ${}^{c}N_L$, ${}^{c}\tau_L$, ${}^{m}N_L$, and ${}^{m}\tau_L$. The measured quantities ${}^{m}N_L$ and ${}^{m}\tau_L$ contain an experimental random measurement error and the computed quantities ${}^{c}N_L$ and ${}^{c}\tau_L$ are in error because of uncertainties in the tabulated gas parameters $\beta_s$ and $k_s$. There are also errors due to deficiencies in the band model used in the gas transmittance calculation. These deficiencies in the model are covered in the references cited in the previous section and will not be covered further here. Thus, even if the computer program succeeds in finding a solution that reduces the residual values to zero, the computed parameters are still in error due to the residual errors. By using equations (6) and (7) it can easily be shown that the residual errors at the solution, $\delta R_N$ and $\delta R_\alpha$ are given by

$$\delta R_N = \frac{\delta {}^{c}N_L}{{}^{c}N_L} - \frac{\delta {}^{m}N_L}{{}^{m}N_L} \tag{20a}$$

$$\delta R_\alpha = \frac{{}^{m}\tau_L}{1 - {}^{m}\tau_L}\left(\frac{\delta {}^{m}\tau_L}{{}^{m}\tau_L} - \frac{\delta {}^{c}\tau_L}{{}^{c}\tau_L}\right) \tag{20b}$$

where $\delta {}^{c}N_L$, $\delta {}^{m}N_L$, $\delta {}^{c}\tau_L$, and $\delta {}^{m}\tau_L$ are the errors in ${}^{c}N_L$, ${}^{m}N_L$, ${}^{c}\tau_L$, and ${}^{m}\tau_L$, respectively.

To proceed further it is necessary to specify the errors in the measured and computed quantities. It will be assumed that all measurements have the same probable error given by $|\delta {}^{m}V/{}^{m}V|$ and that the computed values for $N_L$ and $\tau_L$ have random errors due to the uncertainty $|\delta k_s/k_s|$ in published $k_s$ values.

The uncertainty in the value of $\beta_s$ will be neglected. Thus, only two random errors will be considered, $|\delta^{m}V/^{m}V|$ and $|\delta k_s/k_s|$.

Using equations (10) and the definition ${}^{m}\alpha_L = 1 - {}^{m}\tau_L$ it can be easily shown that

$$\left(\frac{\delta^{m}N_L}{m_{N_L}}\right)^2 = \left(\frac{\delta^{m}V}{m_V}\right)^2 \tag{21a}$$

$$\left(\frac{\delta^{m}\tau_L}{m_{\tau_L}}\right)^2 = 2\left(\frac{\delta^{m}V}{m_V}\right)^2 \tag{21b}$$

$$\left(\frac{\delta^{m}\alpha_L}{m_{\alpha_L}}\right)^2 = 2\left(\frac{\tau_L}{1-\tau_L}\right)^2\left(\frac{\delta^{m}V}{m_V}\right)^2 \tag{21c}$$

To estimate the random errors in the computed quantities, assume a simplified transmittance equation given by ${}^{c}\tau_L = \exp(-kpL)$. It can then be shown that

$$\left(\frac{\delta^{c}N_L}{c_{N_L}}\right)^2 = \left(\frac{\delta^{c}\alpha_L}{c_{\alpha_L}}\right)^2 = \left(\frac{\tau_L \ln \tau_L}{1-\tau_L}\right)\left(\frac{\delta k}{k}\right)^2 \tag{21d}$$

The above quantities when substituted into equations (20a) and (20b) give for the squares of the random residual errors

$$\delta R_N^2 = \left(\frac{\delta^{m}V}{m_V}\right)^2 + \left(\frac{\tau_L \ln \tau_L}{1-\tau_L}\right)^2\left(\frac{\delta k}{k}\right)^2 \tag{22a}$$

$$\delta R_{\alpha}^2 = \left(\frac{\tau_L}{1 - \tau_L}\right)^2 \left[2\left(\frac{\delta^{m_V}}{m_V}\right)^2 + (\ln \tau_L)^2 \left(\frac{\delta k}{k}\right)^2\right] \tag{22b}$$

The random residual error $\delta R_N^2$ (eq. (22a)) depends on the error $\delta k/k$. An alternative form that eliminates this dependence is to substitute for equation (6) the expression

$$\overline{R}_N = ({}^{c}\overline{N}_L - {}^{m}\overline{N}_L)/{}^{m}\overline{N}_L \tag{23}$$

where $\overline{N}_L$ is an apparent radiance defined by

$$\overline{N}_L = N_L/\alpha_L \tag{24}$$

By repeating the previous procedure it can be shown that

$$\delta\overline{R}_N^2 = \left[1 + 2\left(\frac{\tau_L}{1 - \tau_L}\right)^2\right]\left(\frac{\delta^{m_V}}{m_V}\right)^2 \tag{25}$$

The quantity $\delta\overline{R}_N^2$ is less than $\delta R_N^2$ whenever

$$(\ln \tau_L)^2 > \frac{2(\delta^{m_V}/m_V)^2}{(\delta k/k)^2} \tag{26}$$

Because experience has shown that $\delta\overline{R}_N^2$ is less than $\delta R_N^2$ in most practical situations, the computer program presented herein uses $\overline{R}_N$ given by equation (23) instead of $R_N$ given by equation (6) for the residuals in equations (8) or (9).

Equations (25) and (22b) give a measure of the uncertainties in the zero values for the residuals at the solution. These expressions are used in the computer program following the procedure outlined in appendix B to compute the random errors in the temperature and pressure profile parameters.

## Selection of Wavelengths of Measurement

The wavelengths differ principally in their associated gas absorption coefficients. Figure 2 shows the absorption coefficient k for the 2.7 $\mu$m band of $H_2O$. At wavenumbers near the center of the band (3704 $cm^{-1}$), k decreases with temperature; at the wings, k increases with temperature. Substantial differences in k exist, especially at a low temperature. Another difference due to wavelength is caused by a greater increase of the Planck-function radiance with temperature at the shorter wavelengths. Since the variation of k with wavelength is the phenomenon that enables the profile to be determined, large differences would be expected to be favorable.

The wavelengths are selected to maximize accuracy of the solution, and equally important, to avoid an incorrect second solution that can exist. This preliminary selection is performed through an auxiliary computer program WAVES. The selection procedure will be illustrated with both modes of the temperature profile function, equations (1) and (2).

Avoiding an incorrect solution. - The WAVES program uses the following procedure: For assumed values of the two variable temperature parameters in equations (1) or (2), as applicable, and one variable pressure parameter in equation (3), the quantities ${}^{c}\overline{N}_L$ and ${}^{c}\tau_L$ are computed for each wavelength. These computed quantities are substituted for presumed error-free measurements ${}^{m}\overline{N}_L$ and ${}^{m}\tau_L$ of the assumed profiles. Then, taking one wavelength at a time, one parameter w of the temperature profile is assigned a value different from that assumed. The quantities ${}^{c}\overline{N}_L$ and ${}^{c}\tau_L$ change. Then, new values of the other temperature parameter and the pressure parameter are found by iteration that restore the equalities ${}^{c}\overline{N}_L = {}^{m}\overline{N}_L$ and ${}^{c}\tau_L = {}^{m}\tau_L$. This procedure is repeated for a number of assigned values of the temperature profile parameter w, and the results are tabulated by the program.

For each wavelength, the tabulation can be plotted as a curve with the independently varied parameter w as abscissa and the dependent temperature parameter as ordinate. The intersection of any two curves is a two-wavelength solution for a temperature profile.

As an example, assume a path length of 100 cm, hydrogen-air combustion at 1 atm total pressure having $H_2O$ pressure parameters $p_c = 0.35$ atm, $p_w = 0.30$ atm, and $n_p = 0.5$. Computations are made for wavelengths in the 2.7 $\mu$m band of $H_2O$. Results are plotted in figure 3 for the profile of figure 1(a) with $n_T$ as the independent parameter and $T_c$ as dependent, and in figure 4 for the profile of figure 1(b) with $T_w^*$ as the independent parameter and $T_c$ as dependent, with no wall boundary layer ($x_1 = 0$). To facilitate plotting and to emphasize differences in the curves, the ordinate Y of the graph is tabulated by the program as a function

$$Y = Z + \zeta(w - w_o) \tag{27}$$

where Z is the dependent parameter, w is the independent parameter, $w_o$ is the originally-assumed value, and $\zeta$ is chosen by the program as described in appendix C. All curves intersect at the true solution. Some pairs of curves intersect at a second point that is an incorrect solution. For example, in figure 4, wavenumbers 3500 and 3100 $cm^{-1}$ intersect at approximately $T_w^* = 2200$ K and $T_c = 1840$ K. A solution by the computer program converged to $T_w^* = 2223$ K and $T_c = 1873$ K from a starting point $T_w^* = 2300$ K and $T_c = 1800$ K. To assure convergence to the true solution, a pair of curves should have increasing separation with distance from the true solution. Accuracy is greatest when there is a large difference of slope between a pair of curves. Where two curves become parallel, accuracy approaches zero.

Inspection of figures 3 and 4 show that no single pair of wavelengths is satisfactory for all profiles. Acceptable pairs of wavenumbers in figure 3 are (3100, 3550 $cm^{-1}$) and (3100, 3775 $cm^{-1}$). The 2000 K almost-isothermal profile that led to figure 4 shows an acceptable pair

(3500, 3100 $cm^{-1}$) for $T_w^*$ below 2000 K, and an acceptable pair (4100, 3400 $cm^{-1}$) for $T_w^*$ above 2000 K.

Tests of the pressure profile when the two pressure parameters $p_w$ and $p_c$ were assumed to be variables, and only $T_c$ was variable, gave curves nearly alike for all wavelengths. Thus, poor accuracy of the computed pressure profile makes this technique unacceptable; it is therefore necessary to limit oneself to only one variable pressure parameter. The reasons for this poor accuracy are (1) that radiance and absorption coefficient usually vary more strongly with temperature than they do with pressure and (2) that the measurement of $\tau_L$, equation (10) which is the principal source of information about the pressure, is sensitive only to the integral of pressure over the path and not to local values of pressure, whereas $N_L$ (which is the principal source of information about temperature) is sensitive to local temperature.

Maximizing accuracy of the solution. - The program that led to figures 3 and 4 does not provide an estimate of the error for pairs of wavelengths. This estimate is provided by the main program PROFIL (MODE=1). The error estimate is made by pairing one principal wavelength with each of all the other wavelengths to be tested. For each dependent profile parameter, the program tabulates the error in the parameter due to assigned errors of the radiation-measurement voltages $V$ and the tabulated absorption coefficient $k_s$.

As an example, such tabulated values are plotted in figure 5 for the parameter $T_c$ with the profiles and some of the wavelengths of figure 3. The assumed errors were 1 percent in $V$ and 5 percent in $k_s$. Another example with the same assumed error is plotted in figure 6 for $T_c$ with the profiles and some of the wavelengths of figure 4. These errors are for profiles with $T_c$ = 2000 K, and the range of values covered by the abscissa parameter. The errors are consistent with the slope-difference of curve pairs in figures 3 and 4. The error is minimized in figure 6 with wavenumber pairs (4100, 3400 $cm^{-1}$) above 1950 K, and (3500, 3100 $cm^{-1}$) below 1850 K.

All four of these wavenumbers have been used simultaneously in a least squares solution by the program PROFIL (MODE=3). The resulting error also plotted in figure 6(b), shows improvement at all values of $T_w^*$. The effect of path length on the error at $T_w^* = 1200$ and 2000 K is listed in table III, for this four-wavelength combination The error varies approximately as the inverse square root of the path length, in this example.

## PROGRAM DESCRIPTION

The accuracy of the temperature profile found with measured data is dependent on the pressure and temperature profiles, path length, and wavelengths selected for measurement. It is desirable as a preliminary step to assume realistic values for the path length and pressure and temperature profiles for the absorbing gas, and then to select wavelengths and estimate the accuracy of the temperature profile parameters as was illustrated in the Selection of Wavelengths of Measurement section.

A separate main program WAVES (described in "Avoiding an incorrect solution") is designed for the selection of wavelengths. Using these wavelengths, a principal main program PROFIL gives results in three modes of operation:

MODE=1: This program computes the error in the dependent profile parameters that would be caused by assigned random errors of radiometric measurements and tabulated absorption coefficients. For given values of all profile parameters, gas radiance and transmittance are calculated and the parameter errors are computed as in appendix B. Actual radiometric measurements are not required. The estimate may be made for any pair of wavelengths consisting of one "principal" wavelength and any one of up to seven others.

MODE=2: This program computes values for the dependent profile parameters using the iterative procedure described previously. Limits are assigned to the dependent parameters by the user; if a limit is

reached during the iteration, that parameter becomes fixed, and the iteration proceeds for the remaining dependent parameters. When a least-squares solution is used, the magnitude of the final root-mean-square residual R (eq. (9)) is also provided. In addition, using the same procedure as in MODE=1, the error in the dependent parameters that would be caused by assigned random errors in the radiometric measurements and tabulated absorption coefficients is computed.

MODE=3: This program is used to find the change of temperature profile that would be caused by a change in one of the independent profile parameters. A second set of data cards is required that incorporate the change. Starting with an assumed profile and gas-property data, the resulting radiance and transmittance that would be measured are calculated. The second set of data cards is then introduced to change one of the independent profile parameters, and the computation in MODE=2 is performed using the previous radiance and transmittance values to yield a revised profile. This process is useful in identifying independent profile parameters to which the temperature profile is unusually sensitive.

The flowchart for program PROFIL is figure 7. After reading input data and calculating some initial conditions, the main program calls subroutines TEMP that calculates profiles, and TRANS that calculates gas transmittance and radiated flux. The subroutines are principally a computation using equations presented in the text. The equation numbers appear on comment cards in the listings.

The test result DONE=1 is obtained when (1) the number of iterations reaches a preset number, or (2) when the root-mean-square sum of all residuals is less than $10^{-4}$, or (3) when the fractional change of the variable parameters per iterative step has become less than $10^{-4}$ for $T_W$ and $T_c$, and less than $10^{-3}$ for $p_c$ and $n_T$. Criterion (3) is needed when there are more residuals than variable parameters, because the residuals then reach a nonzero minimum.

A subsidiary loop of moderate complexity determines the variable parameter increments and tests the parameters for exceeding their

limits. The loop contains a control index number KEY that manipulates the index of FORTRAN DO statements as follows. The variable profile parameters in equation (1) are $n_T$, $T_c$, $p_c$, $T_w^*$. They are represented by a FORTRAN subscripted variable PA(K) that is controlled by a DO index K=K1, K2, K3. An index initially K=1, 3, 1 selects parameters $n_T$, $T_c$, $p_c$ for the profiles of figure 1(a) and K=2, 4, 1 selects parameters $T_c$, $p_c$, $T_w^*$ for the profiles of figure 1(b).

Any parameter in either profile can be fixed when it reaches an assigned limit by changing the index parameters K1, K2, K3. This is done by setting K1, K2, K3 equal to the subscripted quantities KEY1(KEY), KEY2(KEY), KEY3(KEY) that can be manipulated. The subscript KEY can select any combination of numbers for K1, K2, K3 as shown in table IV. The variable parameters for each KEY are also listed. By designating the profiles of figure 1(a) as PROF=1 and the profiles of figure 1(b) as PROF=2 the table is valid for PROF=1 and PROF=2 when subsequent additions are made, K1=K1-1+PROF, and K2=K2-1+PROF. The initial profile with no limits reached is KEY=1.

Before entering the loop, KEY=1, and K1, K2, K3, are set as in the table. This frees the currently fixed parameters to return inside their limits during every iterative step. Thus, on first entering the loop, all three parameters (corresponding to KEY=1) are incremented and compared with their limits. If the K'th parameter is within its limit, a limit-indicating variable LIM (K4)=0 where K4=K-PROF+1 (to be valid for PROF=1 and PROF=2). If the K'th parameter is outside the limit, LIM(K4)=1. The value of KEY is a number from 1 to 8 given by

$$KEY=1+4*LIM(1)+2*LIM(2)+LIM(3)$$

If this new value of KEY is not 1 or 8 the preceding procedure of this paragraph is repeated only once from the start of the loop with the new value of KEY, and the corresponding K1, K2, K3 to find new parameter increments and tentative new parameter values. The loop is then exited, the tentative new parameter values are then accepted,

and the iteration proceeds. At the solution the error of the profile parameters is estimated. The program listing with a FORTRAN symbol list is appendix D. The subroutine listings are appendixes E and F.

The flow chart for program WAVES is figure 8. After reading the input data, the program (following the procedure described in Selection of Wavelengths of Measurement) first sets ${}^{m}N_L = {}^{c}N_L$ and ${}^{m}\tau_L = {}^{c}\tau_L$ for the initial profile. Then follow three nested loops. An outer DO loop for selecting each given wavelength, a DO loop for assigning given values to one independent variable profile parameter; and an iteration loop like PROFIL that finds the other two dependent variable parameters. If a variable parameter reaches a limit during iteration, the iteration is ended. After completion of the two DO loops the results are tabulated. The program listing, with FORTRAN symbols not used in program PROFIL, is appendix G.

Successive problems in the same run may omit input data that is not changed. (Both PROFIL and WAVES programs.) The READ data is omitted by not putting IREAD=1 in the NAMELIST data. In the NAMELIST, the data-input parameters of temperature, $T_w$, $T_c$, and $n_T$, and pressure, $p_w$, $p_c$, and $n_p$ are given starting values that are not changed by the program because they are replaced by different internal symbols for computation. After computation the values of the internal symbols are printed, but with the corresponding symbols of the initial data-input parameters.

## PROFIL PROGRAM USE

### Input

The input consists of four types of data: (1) computer program control constants (2) measurements of gas radiance and transmittance at selected wavelengths (3) tabulations from the literature of gas transmission parameters at selected wavelengths and (4) independently determined or estimated profiles of partial pressures of the gas reaction products.

The collected input data are read in with a FORTRAN NAMELIST for single-subscript quantities, followed by a FORTRAN READ STATEMENT for multiple-subscript quantities. An example in appendix H shows this input data in the same format as punched on cards, for MODE=1, five wavenumbers, and two gases, $H_2O$ and $N_2$. The data conform to the following specifications.

NAMELIST DATA. - The following list gives the FORTRAN symbol with its subscripted maximum dimension and equivalent algebraic symbol, in the NAMELIST sequence.

| FORTRAN symbol | Algebraic symbol | Description |
|---|---|---|
| MODE | | MODE=1 finds error estimate of pairs of wavenumbers consisting of the first wavenumber paired with each succeeding wavenumber<br>MODE=2 finds solution to given measurements, with error estimate<br>MODE=3 finds gas radiance and transmittance for given input, then requires NAMELIST repeated that may have changes from the first NAMELIST, and finds solution the same as MODE=2 |
| PROF | | PROF=1 profile figure 1(a), variable parameters TC, PC, NT. PROF=2 profile figure 1(b), variable parameters TW, TC, PC, with given boundary layer wall temperature TWB, thickness X(JB) |

| FORTRAN symbol | Algebraic symbol | Description |
|---|---|---|
| IREAD | | IREAD=1 requires READ data for GAS, ALPH, KTAB, BTAB. With IREAD=1 omitted, READ data must be omitted |
| PATH | L | Test section path length, cm |
| I1 (8 maximum) | | Number of wavenumbers for computation (when IREAD=1, I1 must equal number of data cards for KTAB and BTAB) |
| WAVE(8) | $\lambda$ | Wavenumber $cm^{-1}$ |
| MRL(8) | $m_{N_L}$ | Measured radiance W, $cm^{-1}$ $cm^{-2}$ $ster^{-1}$ (eq. (10)) |
| MTAUL(8) | $m_{\tau_L}$ | Measured transmittance (eq. (10)) |
| ERRV | | Percent error of radiation measurement |
| ERRK | | Percent error of tabulated absorption coefficient |
| TW | $T_w$, $T_w^*$ | Gas temperature, K, at wall. For PROF=2 with boundary layer, $T_w^*$ approximates free stream temperature near the wall |
| TC | $T_c$ | Gas temperature, K, on axis |
| NT | $n_T$ | Gas temperature profile equation exponent |
| TWB | $T_w$ | Gas temperature, K, at wall for PROF=2 with boundary layer |

| FORTRAN symbol | Algebraic symbol | Description |
|---|---|---|
| JB (minimum is 1 at wall) | | Index for X(JB) giving distance x from wall where boundary layer ends, for PROF=2 |
| UPLIM(4) | | Upper limit of profile parameters TW, TC, PC, NT |
| BOTLIM(4) | | Lower limit of profile parameters TW, TC, PC, NT |
| L1 (3 maximum) | | Number of absorbing gases |
| L2 (6 maximum) | | Number of absorbing plus non-absorbing gases |
| PS | $p_s$ | Gas static pressure, constant along optical path |
| PC(6) | $p_c$ | Partial pressure of each gas, on axis |
| NP(6) | $n_p$ | Pressure profile equation exponent of each gas |
| PW(6) | $p_w$ | Partial pressure of each gas, at wall |
| NK (8 maximum) | | Number of tabulated values of KTAB read in for data |
| TKTAB(8) | | Temperatures at which values of KTAB are tabulated in READ data |
| NB (8) maximum) | | Number of tabulated values of BTAB read in for data |
| TBTAB(8) | | Temperatures at which values of BTAB are tabulated in READ data |

| FORTRAN symbol | Algebraic symbol | Description |
|---|---|---|
| J1 (41 maximum) | | Number of stations along optical path. Must be odd. Omit if J1=21 in DATA-statement of program is acceptable. |
| Z(J) | | Station distance ratio, from wall to center, as fractional value 0 to 1. Omit if list in DATA-statement of program is acceptable. Maximum J=(J1+1)/2 |
| ITER | | Maximum number of iterations |

READ statement data. - The following list gives the FORTRAN symbol with its subscripted maximum dimension, the format of each card, and the equivalent algebraic symbol.

| FORTRAN symbol | Format | Algebraic symbol | Description |
|---|---|---|---|
| GAS(6) | 6A6 | | Names of all gases |
| ALPH(3, 6) | (12F6.0) | $\alpha^*$ | Broadening factor for up to 3 absorbing gases by up to 6 total number of gases. Card sequence is one card for each L1 absorbing gases. Each card lists the broadening factor for each of L2 gases. |

| FORTRAN symbol | Format | Algebraic symbol | Description |
|---|---|---|---|
| KTAB(8,3,8) | (12F6.0) | $k_o$ | Absorption coefficient at S. T. P. for up to I1=8 wavenumbers, L1=3 gases, NK=8 tabulated points. Card sequence is one set of cards for each of L1 absorbing gases. Each set has I1 cards corresponding to the wavenumbers in NAMELIST. Each card lists absorption coefficients corresponding to temperatures TKTAB in NAMELIST. |
| BTAB(8,3,8) | (12F6.0) | $\beta_o$ | Line-broadening coefficient at S. T. P. for up to I1=8 wavenumbers, L1=3 gases, NB=8 tabulated points. Card sequence same as for KTAB above. Each card lists broadening coefficients corresponding to temperature TBTAB in NAMELIST. |

The two gas transmittance parameters KTAB and BTAB depend on temperature. For $H_2O$ and $CO_2$, they are tabulated in references 10 to 12 with KTAB and BTAB normalized to S. T. P. The program interpolates between tabulated values to find a tabulated value at local temperature, then denormalizes to obtain KK and BB at local temperature and pressure in accordance with equations (18) and (19). Linear interpolation is used. If the profile temperature is outside the temperature range of the tabulation, KK and BB are limited to the extreme tabulated value. It is thus desirable to prepare the tabulation with a temperature range running from the lower to upper limits appearing on other input cards for the profile temperatures TC, TW, and TWB.

## Output

An example of the output shown in appendix H for MODE=1 and PROF=2 consists of four parts:

1. The input NAMELIST and READ data.

2. Estimated error of the profile parameters caused by the residuals, equations (20) and (25), due to the errors of measurement ERRV and of absorption coefficient ERRK. The example has ERRV=1 percent and ERRK=5 percent. The example shows four wavenumbers 3100, 3400, 4100, and 3000 $cm^{-1}$ successively paired with the first wavenumber 3500 $cm^{-1}$. The first pair have residuals $\overline{R}_N = 2.0$ and 3.2 percent at 3500 and 3100 $cm^{-1}$, and $R_\alpha = 4.4$ percent at 3500 $cm^{-1}$. These residuals cause the listed three errors for each parameter, and their rms total.

3. Transmittance at each wavenumber.

4. Temperature and pressure profiles.

An example shown in appendix I for MODE=3 was in the same run and followed the preceding example. The READ statement data and most items in the NAMELIST were not changed. Thus, only two data cards were required. The first four wavenumbers were used in a least squares solution. Appendix I shows the input data in the same format as punched on cards. The first NAMELIST has MODE=3 and I1=4. The required second NAMELIST has a change in the nonvariable pressure parameter, $p_w = 0.36$ replacing $p_w = 0.30$. The output consists of four parts:

1. The first input NAMELIST and the second NAMELIST that differs by the new $p_w = 0.36$ and an internal change to MODE=2. Because IREAD=1 was omitted, the READ data were not required or printed out.

2. Each iteration step lists the parameters, the residuals $\overline{R}_N$ for each wavenumber, the residual $R_\alpha$ for the first wavenumber, the rms total residual, and a step size that is the total fractional change of the variable parameters. In this example the 20 percent change of $p_w$ from 0.30 to 0.36 caused errors $\delta T_c = 1.2$ K or 0.06 percent, $\delta p_c = -0.019$ atm or 5.4 percent, and $\delta T_w = 14$ K or 0.5 percent. Because

four wavenumbers were used (I1=4) the iteration was terminated by the small step size, as the residuals became stationary and remained nonzero.

3. Estimated error of the profile parameters caused by the residuals $\delta R_N$ and $\delta R_\alpha$. The percent errors are $\delta T_c = 3.5$ percent, $\delta p_c = 7.1$ percent and $\delta T_w = 6.6$ percent. These errors are much larger than those listed in (2) above caused by the change of $p_w$.

4. Temperature and pressure profiles.

The output in MODE=2 is the same as MODE=3 without the first NAMELIST.

## WAVES PROGRAM USE

### Input

The input includes all quantities listed for PROFIL. Three additional quantities in the NAMELIST select the independent temperature parameter and assign values to it that differ from the initial value. The independent parameter is determined by index K4 of PA(K4), where K4=1 for $n_T$, K4=2 for $T_c$, and K4=4 for $T_w$. The program selects the dependent parameter in accordance with the profile, either PROF=1 or PROF=2.

| FORTRAN symbol | Description |
|---|---|
| K4 | Index of independent variable temperature parameter PA(K4) |
| NPA | Number of values of PA1 to be used, up to ten. |
| PA1(10) | Values that may be assigned to PA(K4). |

### Output

An example in appendix J shows the input data in the same format as punched on cards for four wavenumbers and two gases, $H_2O$ and $N_2$. The output has four parts:

1. The NAMELIST and READ data
2. Temperature and pressure profiles
3. At each solution found by iteration, the four variable profile parameters, wavenumbers, number of iterations, final rms residual
4. Tabulations of dependent parameter against independent parameter for each solution in (2), with the dependent parameter modified for plotting by equation (27) with the constant $\zeta$

Examples of plotted tabulation are figures 3 and 4.

## DIAGNOSTICS

A warning is printed each time:

1. The pressure of all absorbing gases exceeds the static pressure at any point on the pressure profile.

2. During iteration when a variable parameter reaches the assigned upper or lower limit.

## APPLICATION OF THE PROGRAMS TO AN EXPERIMENT

Three steps are used to determine whether this method will be sufficiently accurate for an application. These steps will be summarized in this section, and an example of an application will be given. The steps are:

1. Estimates of the temperature and pressure profiles are made, and the profile equations are selected.

2. Some wavenumbers for measurement are selected. and then compared using graphs of the output of the WAVES program. This was demonstrated in figures 3 and 4.

3. Accuracy of the dependent profile parameters is determined for the best pairs of wavenumbers selected from graphs in step (2). This was demonstrated in figures 5 and 6. Tests with the PROFIL program in MODE=3 may be run with a perturbation of an independent profile parameter. The resulting change of all dependent profile parameters

may be judged acceptable or excessive. This is demonstrated in appendix I.

Based on the results of steps (2) and (3), it can then be determined if there exists a pair of wavenumbers that lead an acceptably low level of random error in the computed parameters. The experimental measurements are then made at the wavenumbers chosen and the results serve as inputs to the PROFIL program in MODE=2 for determining the temperature and pressure profiles.

An example of the PROFIL program is given to illustrate the limitation of the assumed functional form of the temperature profile as described by two variable parameters. An assumed profile with a high temperature core is shown in figure 9. This profile cannot be matched exactly by equations (1a) or (1b). The pressure profile is the same as used in other examples; hydrogen-air combustion at 1 atm, parameters $p_w = 0.30$ atm, $p_c = 0.35$ atm, and $n_p = 0.50$.

By following steps (1) to (3) given at the beginning of this section it was found that wavenumbers of 3100 $cm^{-1}$ and 3500 $cm^{-1}$ were suitable for use. The radiance and transmittance of the assumed profile were calculated at these wavenumbers to represent error-free measurements. With these measurements as input data, the PROFIL program in MODE=2 found the profiles with equations (1a) and (1b) that are plotted in figure 9. The profiles in figure 9(a) and (c) use an independently determined wall temperature $T_w = 1100$ K that was made 100 K lower than the assumed profile $T_w = 1200$ K. This represents an error of $T_w$. The difference between the assumed and computed profiles is an error of approximation due to limitations in the ability of the profile functions to assume an arbitrary shape. This may be compared with the error band that is due to an assumed radiance measurement error of one percent and a tabulated absorption coefficient error of five percent.

The PROFIL program data cards and output for figure 9(a) are shown in appendix K. The output format is the same as shown and described for MODE=3, appendix I, without the first namelist.

## CONCLUDING REMARKS

All of the examples presented in this report were for hydrogen-air combustion at a pressure of 1 atmosphere with a path length of 100 cm. These reactants produce $H_2O$ as the absorbing gas. It was shown in table III that the random error in the computed profiles decreases with increasing path length. It can also be shown that the random error in the profiles will decrease with increasing pressure or by using a gas with greater absorptance such as $CO_2$. However, in applications where the path length, gas pressure, and gas type are all fixed, a user of this computer program has only the choice of the wavelengths of measurement at his disposal in order to attempt to bring the computed profile errors within acceptable bounds.

# APPENDIX A

## SYMBOLS

| | |
|---|---|
| A | matrix of first derivatives |
| $A_1$ to $A_5$ | coefficients in eqs. (16) and (17) |
| a | element of A |
| B | matrix of second derivatives |
| b | element of B |
| d | average spectral line spacing |
| k | gas absorption coefficient, $cm^{-1}$ |
| L | total path length of profile |
| $n_T$ | exponent in equation for temperature profile |
| $n_p$ | exponent in equation for pressure profile |
| $N_L$ | actual gas radiance |
| m | temperature-gradient, eq. (2) |
| N* | radiance by Planck function |
| $\overline{N}_L$ | apparent radiance defined by eq. (24) |
| p | partial pressure of absorbing gas |
| $p_S$ | static pressure |
| q | number of absorbing gases |
| R | total residual, rms value; also column matrix of residuals |
| R (subscripted) | residual, eq. (6) based on $N_L$ and $\tau_L$ |
| $\delta$R (subscripted) | residual errors, eqs. (20a) and (20b) |
| $\overline{R}$ (subscripted) | residual, eqs. (23), based on $\overline{N}_L$ |
| $\delta\overline{R}$ (subscripted) | residual error, eq. (25) |

| | |
|---|---|
| $T$ | temperature |
| $T_w^*$ | temperature parameter in temperature profile, eq. (2), fig. 2(b) |
| $u$ | dimensionless optical depth |
| $V$ | detector output voltage |
| $w$ | independently varied parameter |
| $x_1$ | boundary layer thickness |
| $x$ | distance along profile or optical path |
| $y$ | dimensionless path-length ratio, eq. (1) or variable parameter, eq. (8), (B1) |
| $Y$ | graph-plotting ordinate, eq. (27) |
| $Z$ | dependent parameter |
| $z$ | dimensionless path-length ratio, eq. (2) |
| $\alpha_L$ | absorption factor of gas |
| $\alpha^*$ | spectral line-broadening coefficient |
| $\beta$ | spectral-line overlap factor, band model parameter |
| $\gamma$ | average spectral line width |
| $\eta$ | interpolation parameter |
| $\lambda$ | wavelength |
| $\rho$ | gas density |
| $\tau_L$ | transmittance |
| $\zeta$ | graph-plotting constant, eq. (27) |

Subscripts:

| | |
|---|---|
| c | centerline of profile |
| s | standard conditions |
| w | ends of profile (wall) |

p pressure

T temperature

N radiance

e effective value

L total path length

$\alpha$ absorptance

$\lambda$ wavelength

o initial conditions

Superscripts:

c computed

m measured

Running indices:

i path length; also wavelength in eq. (6)

j absorbing gases

k nonabsorbing gases; also dependent parameters in matrix solution

$\ell$ intermediate index for path length

# APPENDIX B

## PROFILE PARAMETER ERROR ESTIMATE

In order to use matrix notation and FORTRAN coding, the four variable parameter symbols $T_c$, $T_w$, $p_c$, and $n_T$ are replaced by one subscripted symbol $y_j$. Only three of these are treated as dependent variables at any one time.

Due to random errors in the measured and computed terms that form the residuals $R_N$ and $R_\alpha$, there will also be a random error $\delta y_j$ associated with each parameter $y_j$. The random errors in the residuals are denoted by $\delta R_i$ (see eqs. (20) and (22)).

When the number of equations is equal to the number $m$ of unknowns, the errors $\delta y_j/y_j$ are a solution of $m$ equations in $m$ unknowns,

$$\sum_{j=1}^{m} \frac{\partial R_i}{\partial(\delta y_j/y_j)} \cdot \left(\frac{\delta y_j}{y_j}\right) = \delta R_i \qquad i = 1, m \tag{B1}$$

or, in matrix notation,

$$A\left(\frac{\delta y}{y}\right) = \delta R \tag{B2}$$

The elements of A are partial derivatives in equation (B1) that are found by numerical differentiation in the computer program.

When the number $n$ of equations is greater than the number $m$ of unknowns, the least squares method is applied to give the equation

$$A^T A\left(\frac{\delta y}{y}\right) = A^T \delta R \tag{B3}$$

where $A^T$ is the transpose of A. This can be written as

$$\frac{\delta y}{y} = \left[(A^T A)^{-1} A^T\right]\delta R \tag{B4}$$

which is equivalent to the set of n equations, and m unknowns,

$$\sum_{i=1}^{n} \frac{\partial(\delta y_j/y_j)}{\partial R_i} \cdot \delta R_i = \frac{\delta y_j}{y_j} \tag{B5}$$

Each term in equation (B5) isolates the contributions of $\delta R_i$ to the total error of each variable parameter. Since the sign of $\delta R_i$ is equally likely to be plus or minus, the rms total for all n terms gives the estimated error for each j parameter.

## Damped Least Squares Method

Where an iterative method of solution is used to deduce the profile parameters from experimental measurements, the profile parameter fractional increments are $\delta y_j/y_j$ for an iterative step. The increment size is determined by the residuals $R_i$ which are to be minimized. These residuals are: $\overline{R}_N$, equation (23), at each wavelength $\lambda_i$; $R_\alpha$, equation (7), at wavelength $\lambda_1$. The least squares method, equation (B3), minimizes R by reducing $A^T R$ to zero. Near the solution where $-A^T R$ becomes zero, damping is required to prevent oscillation of the variable parameters about the solution (refs. 17 and 18). When a damping factor is selected in accordance with equation (11) of reference 19, equation (B3) becomes

$$\left[A^T A + (p/q)Q\right]\frac{\delta y}{y} = -A^T R \tag{B6}$$

The elements of matrix A are first derivatives of the residual, given by

$$a_{ij} = y_j(\partial R_i/\partial y_j) \tag{B7}$$

where $R_i$ is by definition a fractional value. The transpose of A is $A^T$. The damping increases the principal diagonal of $A^TA$ by a factor $1 + (p/q)$ where Q is a diagonal matrix whose elements are the principal-diagonal elements of $A^TA$. The number q is the length of the principal-diagonal vector of $A^TA$ whose elements are $q_{i,i}$ so that

$$q = \left( \sum_{\backslash i} q_{i,i}^2 \right)^{1/2} \tag{B8}$$

The number p is the length of a vector given by the matrix product $B^TR$, whose elements are $p_i$, so that

$$p = \left( \sum_{i} p_{i,i}^2 \right)^{1/2} \tag{B9}$$

The elements of B are second derivatives of the residual given by

$$b_{ij} = y_j^2 (\partial^2 R_i / \partial y_j^2) \tag{B10}$$

Finite differences are used to find $a_{ij}$ and $b_{ij}$. First treat the profile parameter $y_1$ as follows for all wavelengths:

(a) Calculate current values of $N_L$ and $\tau_L$

(b) Increase $y_1$ by multiplying it by 1.01

(c) Calculate new values $N_{L,a}$ and $\tau_{L,a}$

(d) Decrease $y_1$ by a factor 0.99/1.01

(e) Calculate new values $N_{L,b}$ and $\tau_{L,b}$

(f) Restore $y_i$ to its starting value by multiplying it by 1/0.99

The first derivatives for the ith wavelength, jth parameter are

$$\left.\begin{aligned} a_{ij} &= ({}^{c}N_{L,b} - {}^{c}N_{L,a})/[0.02(1 - {}^{m}N_{L})] \\ a_{ij} &= ({}^{c}\tau_{L,b} - {}^{c}\tau_{L,a})/[0.02(1 - {}^{m}\tau_{L})] \end{aligned}\right\} \tag{B11}$$

the second derivatives are

$$\left.\begin{aligned} b_{ij} &= -({}^{c}N_{L,a} + {}^{c}N_{L,b} - 2{}^{c}N_{L})/[0.01^{2}(1 - {}^{m}N_{L})] \\ b_{ij} &= -({}^{c}\tau_{L,a} + {}^{c}\tau_{L,b} - 2{}^{c}\tau_{L})/[0.01^{2}(1 - {}^{m}\tau_{L})] \end{aligned}\right\} \tag{B12}$$

Next, repeat the procedure (steps (b) through (f)) for the succeeding profile parameters $y_j$.

# APPENDIX C

## DETERMINATION OF $\zeta$ IN EQUATION (27)

The WAVES program involves the determination of how wavelength $\lambda$ affects the relation between a dependent temperature profile parameter $Z$ and an independent temperature-profile parameter $w$. At the initial value $w_o$, the value of $Z(w_o)$ is invariant with wavelength. However, $Z(w, \lambda)$ changes slightly with wavelength when $w \neq w_o$. The temperature-profile determination depends on these small changes. A graph of $Z$ against $w$ on an ordinary sheet of graph paper would show curves of considerable slope, so that differences between curves for various values of $\lambda$ would not be readily apparent. To exaggerate these differences, the ordinate is changed from $Z$ to $Z + \zeta(w - w_o)$. The value of $\zeta$ is determined as follows.

Let the range of the independent parameter be

$$w_n \leq w \leq w_m$$

Among the values of $Z(w)$ for all the wavelengths which are tried in the computation, there will be a maximum value $Z_{max}(w_n)$ and a minimum value $Z_{min}(w_n)$. Similarly, there will be a maximum value $Z_{max}(w_m)$ and a minimum value $Z_{min}(w_m)$. The value of $\zeta$ is taken as

$$\zeta = \frac{1}{2}\left[\frac{Z_{max}(w_n) + Z_{min}(w_n)}{2(w_n - w_o)} + \frac{Z_{max}(w_m) + Z_{min}(w_m)}{2(w_m - w_o)}\right] \qquad (C1)$$

The total span of ordinate values is thereby reduced severalfold.

# APPENDIX D

## PROFIL PROGRAM

### Program Symbols

The following FORTRAN symbol list includes symbols in the subroutines of appendixes E and F. It does not include symbols defined for NAMELIST and READ data in the section PROFIL PROGRAM USE.

| FORTRAN symbol | Description |
|---|---|
| A(5,5) | Condensed matrix of first derivatives |
| B(4) | Condensed matrix of second derivatives |
| BB(8,3,41) | Denormalized and broadened BO |
| BE(8,3,41) | BB weighted by KK |
| BO(8,3,21) | Interpolated local value of BTAB |
| CP(6,41) | Constant of pressure profiles; ratio of each absorbing gas pressure to first absorbing gas pressure; ratio of each nonabsorbing gas pressure to the total pressure of nonabsorbing gases |
| C1 | Constant of pressure profile of first absorbing gas, PW(1)/PC(1) |
| DAMP | Damping constant for diagonal of least squares matrix |
| DEL(4) | Fractional change of variable parameter for derivatives (in data statement) |
| DPA(4) | Variable parameter increment for iteration step |
| DPAPA(4) | Fractional value of DPA |

| FORTRAN symbol | Description |
|---|---|
| DPV(3) | DPA in condensed matrix |
| DTAU(8, 41) | Increment in transmittance |
| DUM | Dummy to prevent overflow or underflow |
| DUM1 | Dummy to prevent overflow or underflow |
| DUM2 | Dummy to prevent overflow or underflow |
| DX(41) | Distance between stations X along path |
| ERR(10) | Residual caused by errors ERRV and ERRK |
| ETA(8, 3, 41) | Interpolation parameter |
| G(10, 6) | First derivatives for least squares matrix |
| GSAV(8, 4) | Dummy variable equal to G |
| GV(9, 5) | Dummy variable equal to G in condensed matrix |
| H(9, 5) | Second derivatives for damping least squares matrix |
| HV(9, 5) | Dummy variable equal to H |
| IA | Index parameter equal to I |
| IB | Index parameter equal to I1 |
| ITER1 | Iteration counter |
| I2 | Wavenumber index parameter I+1 |
| JMIR | Index for reflection of profile about center |
| J2 | Path index parameter (J1+1)/2 |
| J3 | Path index parameter J1+1 |
| KO(8, 3, 21) | Interpolated local value of KTAB |
| KEY | Selector for variable parameters |

| FORTRAN symbol | Description |
|---|---|
| KEY1(8) | Index parameter (data statement) |
| KEY2(8) | Index parameter (data statement) |
| KEY3(8) | Index parameter (data statement) |
| KK(8, 3, 41) | Denormalized KO |
| KV | Index of condensed matrix |
| KV2 | Index parameter KV+2 |
| K1 | Index parameter for variable parameters |
| K2 | Index parameter for variable parameters |
| K3 | Index parameter for variable parameters |
| LX | Index parameter for error array |
| L3 | Index parameter for gas type |
| MAX | Largest absolute value of all DPAPA for an iteration step |
| NEWLIM | Controls number of tests for upper and low parameter limits |
| NP1 | Equals pressure profile equation exponent NP(1) |
| NTEST | Diagnostic indicator of absorbing gas pressure being greater than static |
| P(6, 41) | Pressure of each gas at each station along path |
| PAERR(4, 10) | Error of variable parameter caused by a residual ERR |
| PA1(4) | Tentative value of new PA for an iterative step |
| PSUM | Sum of pressure of all absorbing gases along path |

| FORTRAN symbol | Description |
|---|---|
| R(8, 41) | Gas radiance |
| RA(8) | Equals CRL during numerical differentiation |
| RAB(8) | Equals CRL before numerical differentiation |
| RB(8) | Equals CRL during numerical differentiation |
| R1(8) | Constant of Planck equation |
| R2(8) | Constant of Planck equation |
| STEP | Sum of fractional changes to variable parameters for an iteration step |
| T(41) | Temperature at each station along path |
| TAU(8, 4, 41) | Transmittance at each station along path |
| U(8, 3, 41) | Optical depth at each station along path |
| WAVOUT(10) | Wavenumbers in sequence for printout |
| X(41) | Actual path lengths Z· PATH/2 |
| Y(21) | Dummy equal to Z, the normalized path length |

PROFILE Program Listing

```
00101     1*          COMMON PROF,TWB,   L1,J1,J2,J3,C1,PSUM,JB,R1(8),R2(8),X(41),
00101     2*         X PA(4),CTAUL(8),CRL(8),T(41),DX(41),NK,NE,PS,PATH,L2, Y(21),L3,
00101     3*         X DTAU(8,41),R(6,41),CP(6,41),P(6,41),ALPH(3,8),
00101     4*         X TKTAB(    8),KTAB(8,3,8),KO(8,3,21),KK(9,3,41),IBTAB(8),
00101     5*         X BTAB(8,3,8),BO(6,3,21),BP(8,3,41),BE(8,3,41),ETA(8,3,41),
00101     6*         X U(8,3,41),TAU(8,4,41),NP1,IA,IB,NTEST,TX
00103     7*          REAL KK,KTAB,KO,NP1
00104     8*          INTEGER PROF,DONE
00105     9*          DIMENSION DPAPA(4),RAB(8),DPA(4),KEY1(8),KEY2(8),KEY3(8),DEL(4),
00105    10*         X RA(8),RB(8),G(4),DPV(3),PA1(4),BOTLIM(4),UPLIM(4),LIM(4),MRL(8),
00105    11*         X MTAUL(8),G(10,6),H(9,5),GV(9,5),HV(9,5),A(5,5),PAERR(4,10)
00105    12*         X ,SAS(6),WAVE(6),Z(21),ERR(10),WAVOUT(10),GSAV(8,4),PW(6),NP(6),
00105    13*         X PC(6)
00106    14*          REAL MTAUL,MRL,MT,NP,MAX
00107    15*          NAME LIST/NAM1/MODE,PROF,IREAD,PATH,I1,WAVE,MRL,MTAUL,
00107    16*         X ERRV,ERRK,TW,TC,NT,TWB,JB,UPLIM,BOTLIM,L1,L2,PS,PC,NP,PW,NK,
00107    17*         X TKTAB,NB,TBTAB,J1,Z,ITER,TX
00110    18*          DATA KEY1/4*1,2,2,3,3/,KEY2/3,2,3,1,3,2,3,3/,KEY3/1,1,2,4*1,3/
00110    19*         X ,DEL/4*.01/,J1/21/,Z/0.,.01,.02,.05,.1,.2,.3,.4,.5,.7,1.,10*1./
00116    20*    600 IREAD=0
00117    21*          READ(5,NAM1,END=999)
00120    22*          IF(IREAD.EQ.0)GO TO 67
00123    23*          READ(5,80)(GAS(L),L=1,6)
00125    24*          READ(5,81)(((ALPH(L,LL),LL=1,B ),L=1,L1)
00130    25*          READ(5,81)(((KTAB(I,L,N),N=1,8),I=1,I1),L=1,L1)
00141    26*          READ(5,81)(((BTAB(I,L,N),N=1,8),I=1,I1),L=1,L1)
00155    27*          DO 65 L=1,L1
00171    28*          ALPH(L,L)=1.
00174    29*          DO 65 I=1,I1
00175    30*          DO 68 N=1,NK
00200    31*       68 IF(KTAB(I,L,N).LT. .1E-06)KTAB(I,L,N)=.1E-06
00203    32*          DO 66 N=1,NB
00206    33*       66 IF(BTAB(I,L,N).LT. .1E-06)BTAB(I,L,N)=.1E-06
00211    34*       67 CONTINUE
00216    35*          WRITE(6,90)
00217    36*          WRITE(6,NAM1)
```

```
      IF(IREAD.EQ.0)GO TO 622
      WRITE(6,66) (GAS(L),L=1,6)
      WRITE(6,67)(((ALPHA(L,LL),LL=1,8),L=1,L1)
      WRITE(6,68)(((KTAB(I,L,N),N=1,8),I=1,11),L=1,L1)
      WRITE(6,69)(((BTAB(I,L,N),N=1,8),I=1,11),L=1,L1)
C     INITIAL CONDITIONS
      NTEST=0
  622 IA=1
      IB=I1
      DONE=0
      ITER=0
      DAMP=0.
      I2=I1+1
      J3=J1+1
      J2=(J1+1)/2
      L3=L1+1
      C1=Pw(1)/PC(1)
      PA(1)=NT
      PA(2)=TC
      PA(3)=PC(1)
      PA(4)=TW
      DO 64 K=1,4
      DPAPA(K)=0.
      DPA(K)=0.
      CTAUL(K)=0.
      CTAUL(K+1)=0.
      DO 64 I=1,10
      WAVOUT(I)=0.
      ERR(I)=0.
      S(I,K)=0.
      S(I,5)=0.
   64 PAERR(K,I)=0.
      DO 50 I=1,I1
      IF(MODE.EQ.1)GO TO 65
      WAVOUT(I)=WAVE(I)
      WAVOUT(I2)=WAVE(I)
   65 R1(I)= .11909E-11 *WAVE(I)**3
   50 R2(I)=1.4388*WAVE(I)
      DO 51 J=1,J2
      JMIR=J3-J
      X(J)=PATH*Z(J)/P.
      Y(J)=Z(J)
   51 X(JMIR)=PATH-X(J)
      DO 59 J=2,J1
   59 DX(J)=X(J)-X(J-1)
C     PRESSURE PROFILE INITIAL PROFILES
      NP1=NP(1)
      DO 52 J=1,J2
      DO 53 L=1,L2
      DUM1=ABS(PC(L)-Pw(L))
      P(L,J)=PC(L)
      IF(DUM1.EQ.0..OR.J.EQ.J2)GO TO 53
      DUM=1.-Y(J)
      DUM2=ALOG(DUM1)+ALOG(DUM)/NP(L)
      IF(DUM2.LT. -50.)GO TO 53
   58 P(L,J)=PC(L)-(PC(L)-Pw(L))*DUM**(1./NP(L))
   53 CONTINUE
```

```
                      IF(L1.EQ.1)GO TO 55                                       000410
                C     PRESSURE PROFILE RATIO FACTORS CP(L,J)                    000410
                      DO 54 L=2,L1                                              000412
                   54 CP(L,J)=P(L,J)/P(1,J)                                     000420
                      IF(L2.EQ.L1)GO TO 52                                      000424
                      DUM=0.                                                    000426
                      DO 56 L=L1,L2                                             000432
                   56 DUM=DUM+P(L,J)                                            000442
                      DO 57 L=L1,L2                                             000451
                   57 CP(L,J)=P(L,J)/DUM                                        000451
                   52 CONTINUE                                                  000460
                      IF(MODE.EQ.2)GO TO 701                                    000460
                      CALL TEMP                                                 000463
                      CALL TRANS                                                000465
                      DO 63 I=1,I1                                              000472
                      MRL(I)=CRL(I)                                             000672
                   63 MTAUL(I)=CTAUL(I)                                         000673
                      IF(MODE.EQ.1)GO TO 701                                    000676
                      MODE=2                                                    000701
                      GO TO 600                                                 000703
                  701 WRITE(6,91)(PA(I),I=1,4),PW(1),NP(1)                      000705
                C     BEGIN ITERATION LOOP                                      000720
                  700 CALL TEMP                                                 000721
                      CALL TRANS                                                000723
                      IF(NTEST.EQ.1)WRITE(6,77)                                 000733
                      NTEST=0                                                   000733
                C     FIND RESIDUALS, TEST FOR SOLUTION OR MAXIMUM ITERATION NUMBER  000733
                      RESID=0.                                                  000734
                      TAJA=CTAUL(1)                                             000735
                      DO 1 I=1,I1                                               000745
                      RA=I)=CRL(I)                                              000746
                      S(1,5)=CRL(I)/MRL(I)-1.                                   000746
                    1 RESID=RESID+S(1,5)**2                                     000751
                      IF(MODE.EQ.1)GO TO 406                                    000755
                      S(I2,5)=(MTAUL(I)-CTAUL(I))/(1.-MTAUL(I))                 000760
                      RESID=SQRT(RESID+S(I2,5)**2)                              000766
                      STEP=0.                                                   000775
                      DO 2 J=1,4,2                                              001001
                      STEP=STEP+ABS(DPA=A(J))*.1                                001001
                    2 STEP=STEP+ABS(DPA=A(J+1))                                 001004
                      IF((ITER1.GT.0).AND.(STEP.LT..0001.OR.ITER1.EQ.ITER.OR.RESID.LT.  001010
                     X .0001))DONE=1                                            001010
                      WRITE(6,52)(DPA(I),I=1,4),ITER1,RESID,STEP,(PA(I),I=1,4),  001044
                     X (S(I,5),I=1,5),(WAVOUT(I),I=1,5)                         001044
                      ITER1=ITER1+1                                             001071
                C     DERIVATIVES EQ(P11, 312)                                  001071
                  406 KEY=1                                                     001075
                      K1=KEY1(KEY)-1+PROF                                       001076
                      K2= KEY2(KEY)-1+PROF                                      001103
                      K3=KEY3(KEY)                                              001107
                      DEL(1)=.01/PA(1)                                          001111
                      DO 3 K=K1,K2,K3                                           001234
                      PA(K)=PA(K)*(1.+DEL(K))                                   001241
                      CALL TEMP                                                 001245
                      CALL TRANS                                                001247
                      DO 4 I=1,I1                                               001254
                    4 RA(I)=CRL(I)                                              001254
```

```
                  TAJA=CTAUL(I)                                                 001756
                  PA(K)=PA(K)*(1.-DEL(K))/(1.+DEL(K))                           001760
                  CALL TEMP                                                     001767
                  CALL TRANS                                                    001771
                  DO 5 I=1,I1                                                   001776
                5 RB(I)=CR_(I)                                                  001776
                  TAJB=CTAUL(I)                                                 001780
                  PA(K)=PA(K)/(1.-DEL(K))                                       001782
                  DO 6 I=1,I1                                                   001712
                  G(I,4)= (RA(I)-RB(I))/(2.*DEL(K)*MRL(I))                      001712
                  GSAV(I,K)=G(I,K)                                              001717
                6 H(I,4)= (RA(I)+RB(I)-2.*RAR(I))/(DEL(K)**2*MRL(I))           001721
                  G(I2,K)=(TAUA-TAJA)/(2.*DEL(K)*(1.-MTAUL(I)))                 001333
                  H(I2,K)=(TAUA+TAJB-2.*TAJAR)/(DEL(K)**2*(1.-MTAJL(I)))        001742
                5 CONTINUE                                                      001765
                  CALL TEMP                                                     001765
                  CALL TRANS                                                    001767
                  NEWLIM=0                                                      001771
                  DO 32 K=1,4                                                   001427
                  PA1(K)=PA(K)                                                  001427
               32 LIM(K)=0                                                      001430
               C  FOR MODE=1, SEQUENTIALLY SHIFT DERIVATIVES ABOVE I=2 TO I=2   001430
                  DO 401 M1=2,I1                                                001435
                  IF(MODE.NE.1)GO TO 500                                        001461
                  I2=3                                                          001463
                  WAVOUT(1)=WAVE(1)                                             001465
                  WAVOUT(2)=WAVE(M1)                                            001467
                  WAVOUT(3)=WAVE(1)                                             001471
                  DO 402 K=K1,K2,K3                                             001510
                  G(3,4)=G(I1+1,K)                                              001510
               402 G(2,4)=GSAV(M1,K)                                            001511
               500 CONTINUE                                                     001515
               C  CHANGE DERIVATIVE VARIABLES TO CONDENSE ARRAY K=K1,K2,K3 TO K=1,KV  001515
                  KV=0                                                          001515
                  DO 7 K=K1,K2,K3                                               001563
                  KV=KV+1                                                       001563
                  DO 7 I=1,I2                                                   001566
                  GV(I,KV)=G(I,K)                                               001563
                7 HV(I,KV)=H(I,K)                                               001564
               C  LEAST SQUARES MATRIX AT--A EQ(86)                             001564
                  DO 8 I=1,KV                                                   001576
                  DO 8 K=1,KV                                                   001614
                  A(I,K)=0.                                                     001614
                  DO 8 J=1,I2                                                   001616
                8 A(I,K)=A(I,K)+GV(J,K)*GV(J,I)                                 001616
                  IF(MODE.EQ.1)GO TO 403                                        001637
               C  RESIDUAL VECTOR BT--R EQ(86) AND DAMPING VECTOR  D  EQ(86)    001637
                  KV2=KV+2                                                      001642
                  DO 9 K=1,KV                                                   001645
                  A(K,KV2)=0.                                                   001656
                  B(K)=0.                                                       001656
                  DO 9 J=1,I2                                                   001662
                  A(K,KV2)=A(K,KV2)-GV(J,K)*G(J,5)                              001662
                9 B(K)=B(K)+HV(J,K)*G(J,5)                                      001665
                  DAMPE=0.                                                      001732
                  IF(I2.EQ.KV.OR.DONE.EQ.1)GO TO 12                             001763
               C  NORMALIZED DAMPING VECTOR P/L  EQ(88, 89)  AND DAMPED MATRIX  001763
```

```
                D1=0.                                                   001712
                D2=0.                                                   001713
                DO 10 K=1,KV                                            001723
                D1=D1+A(K,K)**2                                         001723
             10 D2=D2+B(K)**2                                           001726
                DAMP=SQRT(D2/D1)                                        001733
                DO 11 K=1,KV                                            001741
             11 A(K,K)= A(K,K)*(1.+DAMP)                                001746
             12 CONTINUE                                                001752
      C         INVERSE OF LEAST SQUARES MATRIX  AT--A                  001752
            403 NQ=KV+1                                                 001752
                DO 13 I=1,KV                                            001754
                DO 14 J=1,KV                                            002033
             14 A(J,NQ)=0.                                              002033
                A(I,NQ)=1.                                              002034
                DIV=A(I,I)                                              002036
                DO 15 J=1,NQ                                            002042
             15 A(I,J)= A(I,J)/DIV                                      002042
                DO 16 J=1,KV                                            002051
                IF(I.EQ.J)GO TO 16                                      002054
                FAC=A(J,I)                                              002057
                DO 17 K=1,NQ                                            002067
             17 A(J,K)=A(J,K)-A(I,K)*FAC                                002067
             16 CONTINUE                                                002102
                DO 18 J=1,KV                                            002102
             18 A(J,I)=A(J,NQ)                                          002102
             13 CONTINUE                                                002116
                IF(DONE.EQ.1.OR.MODE.EQ.1) GO TO 404                    002116
      C         SOLVE FOR PARAMETER FRACTIONAL INCREMENTS A-INVERSE*AT--R 002116
                DO 19 I=1,KV                                            002137
                DPV(I)=0.                                               002137
                DO 19 K=1,KV                                            002143
             19 DPV(I)=DPV(I)+A(I,K)*A(K,KV2)                           002143
      C         EXPAND INDEX TO ORIGINAL PARAMETER INDEX K=K1,K2,K3     002143
                KV=0                                                    002155
                DO 20 K=K1,K2,K3                                        002164
                KV=KV+1                                                 002164
                DPAPA(K)=DPV(KV)                                        002166
             20 DPA(K)= DPAPA(K)*PA(K)                                   002171
      C         PROPORTIONALLY REDUCE PARAMETER STEP SIZE FOR LARGEST STEP .1*PA 002171
      C         OR .1 FOR PA(1)                                         002171
                MAX=0.                                                  002174
                DO 21 K=K1,K2,K3                                        002200
                DUM=ABS(DPAPA(K))                                       002200
                IF(K.EQ.1)DUM=ABS(DPA(1))                               002202
             21 IF(DUM.GT.MAX)MAX=DUM                                   002207
                IF(MAX.LT..1)MAX=.1                                     002217
                DO 22 K=K1,K2,K3                                        002233
             22 PA1(K)=PA(K)+DPA(K)*.1/MAX                              002233
      C         TEST FOR TENTATIVE PARAMETERS OUTSIDE LIMIT             002237
                DO 23 K=K1,K2,K3                                        002243
                K4=K+1-PROF                                             002243
                IF(PA1(K).GE.BOTLIM(K))GO TO 24                         002247
                PA1(K)=BOTLIM(K)                                        002253
                WRITE(6,83)K,PA1(K)                                     002255
                LM(K4)=1                                                002264
             24 IF(PA1(K).LE.UPLIM(K))GO TO 23                          002270
```

```
                PA(K)=UPLIM(K)                                                  002773
                WRITE(6,,?)K,PA(K)                                              002775
                LIM(K4)=1                                                       002784
             27 CONTINUE                                                        002711
                NEWLIM=NEWLIM+1                                                 002711
                IF(NEWLIM .EQ. 2) GO TO 28                                      002714
                KEY=1+4 *LIM(1)+2 *LIM(2)+LIM(3)                                002716
                K1=KEY1(KEY)-1+PROF                                             002726
                K2= KEY2(KEY)-1+PROF                                            002733
                K3=KEY3(KEY)                                                    002737
                IF(KEY.EQ.1 .OR. KEY.EQ.8) GO TO 26                             002741
                GO TO 29                                                        002754
C       ACCEPT LIMITS AND TENTATIVE PARAMETERS                                  002754
             26 DO 27 K=1,4                                                     002760
                DPA(K)=PA1(K)-PA(K)                                             002760
                DPAPA(K)=DPA(K)/PA(K)                                           002762
             27 PA(K)=PA1(K)                                                    002764
                GO TO 7?6                                                       002767
C       PARAMETER ERROR ESTIMATE                                                002767
            4?4 DO 33 I=1,I1                                                    002771
             33 ERR(I)=SQRT(1.+2.*CTAUL(I)/(1.-CTAUL(I)))*ERRV                  002774
                ERR(I?)=((CTAUL(1)/(1.-CTAUL(1)))*SQRT(2.*ERRV**2+(ALOG(CTAUL.1))
               X *ERRK)**?)                                                     002410
                IF(MODE.NE.1)GO TO 34                                           002412
                ERR(2)=SQRT(1.+2.*CTAUL(M1)/(1.-CTAUL(M1)))*ERRV                002415
                ERR(4)=0.                                                       002431
                ERR(5)=0.                                                       002432
                ERR(6)=0.                                                       002433
             34 DO 29 L=1,3                                                     002435
                LX=L-1+PROF                                                     002445
                PAERR(LX,6)=0.                                                  002447
                DO 30 I=1,I2                                                    002460
                PAERR(LX,I)=0.                                                  002460
                DO 31 K=1,3                                                     002464
                JX=K-1+PROF                                                     002464
             31 PAERR(LX,I)=PAERR(LX,I)+A(L,K)*G(I,J)*ERR(I)                    002470
             30 PAERR(LX,6)=PAERR(LX,6)+PAERR(LX,I)**?                          002501
             29 PAERR(LX,6)=SQRT(PAERR(LX,6))                                   002517
                PSUM=0.                                                         002524
                DO 59 L=1,L1                                                    002531
             59 PSUM=PSUM+P(L,J?)                                               002531
                IF(PSUM.GT.PS)WRITE(6,?7)                                       002534
                WRITE(6,?4) ((PAERR(L,I),L=1,4),WAVOUT(I),ERR(I),I=1,6)         002546
            401 IF(MODE.NE.1)GO TO 407                                          002565
            407 CONTINUE                                                        002573
                WRITE(6,?61)(WAVE(I),I=1,8),(CTAUL(I),I=1,8),(GAS(L),L=1,6),    002573
               X (X(J),T(J),(P(I,J),I=1,6),J=1,J1)                              002573
                GO TO 600                                                       002626
             7[ FORMAT (5?H ASSUMING GAS PRESSURE GREATER THAN STATIC PRESSURE  ) 002630
             ?? FORMAT(4A4)                                                     002630
             ?1 FORMAT ( 8F6.?)                                                 002630
             ?2 FORMAT(1H?/1H0,14HINCREMENTS DPA ,F9.3,F9.2,F9.5,F9.2,4X,       002630
               X 12HITERATION= ,I?,7X,13HRMS RESIDUAL= ,E8.3,7H  STEP= ,E8.3    002636
               X                  /1H0,14HPARAMETERS  PA ,F9.5,F9.2,F9.5,F9.2,4X, 002630
               X 12HRESIDUALS= 6E10.3/48X,17HWAVENUMBER(1/CM)= ,8F10.?)         002630
             ?3 FORMAT(1H?,17HLIMIT REACHED,PA(,I1,2H)= ,F9.3)                  002655
             ?4 FORMAT(1H?/   1X,15HPARAMETER ERROR,3?X,16HWAVENUMBER(1/CM),2X,  002630
               X16HRESIDUAL,PERCENT/1X,8HPERCENT ,7X,4(F6.1,1H%),F11.?,9X,F6.1,1H% 002630
               X/4(19X,4F6.1,F12.?, 9X,F6.1/)6X,9HRMS TOTAL ,4F9.1,F12.6, 9X,F6.1) 002630
             ?5 FORMAT(1H?,5H GAS , 6(4X,A6))                                   002630
             ?7 FORMAT(1H?,5HALPHA ,8F10.2/(6X,8F10.2))                         002630
             ?8 FORMAT(1H?,5HKTABS ,8F10.4/(6X,8F10.4))                         002630
             ?9 FORMAT(1H?,5HETABS ,8F10.?/(6X,8F10.3))                         002630
             91 FORMAT(1H1)                                                     002630
             91 FORMAT(1H1,7X,7HPROFILE,5X,4HTEMP,4X,5HAXIAL,4X,5HAXIAL,5X,4HWALL, 002630
               X1?X,4HWALL,4X,5HPRESS/5X,10HPARAMETERS,7X,8HEXPONENT,3X,4HTEMP,4X, 002630
               X5HPRESS,5X,4HTEMP,14X,5HPRESS,3X,8HEXPONENT/21X,2HNT,6X,4HTC,K,4X, 002630
               X5HPRESS,ATM,4X,4HTW,K,14X,6HPW,ATM,4X,2HAP/17X,F9.5,F9.2,F9.5,F9.2, 002630
               X 9X,2F9.5)                                                      002630
            3?1 FORMAT (1?HWAVENUMBER(1/CM)= ,8F9.?/1?H    TRANSMITTANCE ,      002630
               X8F8.3/ 1H0,19HTEMPERATURE PROFILE, 5X,28HPARTIAL PRESSURE PROFILES 002630
               X (ACH GAS,ATM  /4X,4HX,6M,4X,5HTEMP,K ,6(3X,1A6)//(3(1X,F7.2,F10.2 002630
               X,6F9.4)))                                                       002630
            999 STOP                                                            002630
                END                                                             002633
```

# APPENDIX E

## TEMP SUBROUTINE LISTING

```
00101     1*          SUBROUTINE TEMP                                                    000012
00102     2*          COMMON PROF,TWB,   L1,J1,J2,J3,C1,PSUM,JB,R1(8),R2(8),X(41),       000012
00103     3*         X PA(4),CTAUL(8),CRL(8),T(41),DX(41),NK,NB,PS,PATH,L2, Y(21),L3,    000012
00104     4*         X CTAU(8,41),R(8,41),CP(6,41),P(6,41),ALPH(3,8),                    000012
00105     5*         X TKTAB(    8),KTAB(8,3,8),KO(8,3,21),KK(8,3,41),TGTAB(8),         000012
00106     6*         X BTAB(8,3,8),BO(8,3,21),BB(8,3,41),BE(8,3,41),ETA(8,3,41),        000012
00107     7*         X U(8,3,41),TAU(8,4,41),NP1,IA,IB,NTEST,TX                         000012
00108     8*          REAL KK,KTAB,KO,NP1                                               000012
00109     9*          INTEGER PROF                                                      000012
00110    10*     C    TEMP AND PRINCIPAL PRESSURE PROFILE EQ(1 ,2, 3)                   000012
00106    11*          PW1=PA(3)*C1                                                      000012
00107    12*          DUM1=ABS(PA(2)-PA(4))                                             000031
00110    13*          DUM2=ABS(PA(3)-PW1)                                               000037
00111    14*          DO 1 J=1,J2                                                       000042
00114    15*          JMIR=J3-J                                                         000056
00115    16*          T(J)=PA(2)                                                        000061
00116    17*          DUM=1-Y(J)                                                        000063
00117    18*          IF(DUM1.EQ.0..OR.J.EQ.J2)GO TO 11                                 000066
00121    19*          DUM3=ALOG(DUM1)+ALOG(DUM)/PA(1)                                   000075
00122    20*          IF(DUM3.LT.-80.)GO TO 2                                           000107
00124    21*       11 T(J)=PA(2)-(PA(2)-PA(4))*DUM**(1./PA(1))                          000113
00125    22*        2 IF(Y(J).GT. .51) T(J)=T(J)+TX*(SIN(3.1416*(Y(J)-.5)))**2          000122
00127    23*          T(JMIR)=T(J)                                                      000142
00130    24*          P(1,J)=PA(3)                                                      000145
00131    25*          IF(DUM2.EQ.0..OR.J.EQ.J2)GO TO 1                                  000147
00133    26*          DUM3=ALOG(DUM2)+ALOG(DUM)/NP1                                     000156
00134    27*          IF(DUM3.LT.-80.)GO TO 1                                           000170
00135    28*       12 P(1,J)=PA(3)-(PA(3)-PW1    )*DUM**(1./NP1)                     000173
00137    29*        1 P(1,JMIR)=P(1,J)                                                000203
00137    30*     C    PRESSURE PROFILE OF OTHER ABSORBING GASES                         000203
00141    31*          DO 3 J=1,J2                                                       000210
00144    32*          JMIR=J3-J                                                         000224
00145    33*          PSUM=0.                                                           000231
00146    34*          IF(L1.EQ.1)GO TO 4                                                000232
00150    35*          DO 5 L=2,L1                                                       000234
00153    36*          P(L,J)=P(1,J)*CP(L,J)                                             000244
00154    37*          P(L,JMIR)=P(L,J)                                                  000246
00155    38*        5 PSUM=PSUM+P(L,J)                                                  000247
00157    39*        4 PSUM=PSUM+P(1,J)                                                  000254
00157    40*     C    PRESSURE PROFILE OF NON ABSORBING GASES                           000254
00160    41*          IF(L2.EQ.L1)GO TO 3                                               000264
00162    42*          DUM=PS-PSUM                                                       000267
00163    43*          IF(DUM.LT.0.)DUM=0.                                               000276
00165    44*          DO 7 L=L3,L2                                                      000310
00170    45*          P(L,J)=DUM*CP(L,J)                                                000310
00171    46*        7 P(L,JMIR)=P(L,J)                                                  000312
00173    47*        3 IF(PSUM.GT.PS)NTEST=1                                             000316
00173    48*     C    TEMPERATURE BOUNDARY LAYER,WALL TEMPERATURE TWB                   000316
00176    49*          IF(JB.LE.1.OR.PROF.EQ.1)GO TO 9                                   000327
00200    50*          DO 8 J=1,JB                                                       000344
00203    51*          JMIR=J3-J                                                         000356
00204    52*          DUM=(T(J2)-T(JB))/(PA(1)*(1.-Y(JB)))                              000361
00205    53*          DUM0=Y(J)/Y(JB)                                                   000366
00206    54*          T(J)=TWB+(T(JB)-TWB)*DUM3+(DUM*Y(JB)+TWB-T(JB))*DUM3*(DUM3-1.)    000371
00207    55*        8 T(JMIR)=T(J)                                                      000406
00207    56*     C    RADIANCE PROFILE FOR I  WAVELENGTHS,PLANCK FUNCTION               000406
00211    57*        9 DO 10 J=1,J2                                                      000412
00214    58*          JMIR=J3-J                                                         000420
00215    59*          DO 10 I=IA,IB                                                     000423
00220    60*          DUM=R2(I)/T(J)                                                    000433
00221    61*          IF(ABS(DUM).GT.80.)DUM=80.                                        000435
00223    62*          R(I,J)=R1(I)/(EXP(DUM)-1.)                                        000443
00224    63*       10 R(I,JMIR)=R(I,J)                                                  000452
00227    64*          RETURN                                                            000462
00230    65*          END                                                               000523
```

# APPENDIX F

## TRANS SUBROUTINE LISTING

```
00171     1*          SUBROUTINE TRANS                                                  000126
00172     2*          COMMON PROF,TWB,   L1,J1,J2,J3,C1,PSUM,JB,R1(8),R2(8),X(41),      000126
00173     3*         X PA(4),CTAUL(8),CRL(8),T(41),DX(41),NK,NB,PS,PATH,L2, Y(21),L3,   000126
00174     4*         X CTAU(8,41),R(8,41),CP(6,41),P(6,41),ALPH(3,8),                   000126
00175     5*         X TKTAB(    8),KTAB(8,3,8),KO(8,3,21),KK(8,3,41),TBTAB(8),        000126
00176     6*         X BTAB(8,3,8),BO(8,3,21),BR(8,3,41),BE(8,3,41),ETA(8,3,41),       000126
00177     7*         X U(8,3,41),TAU(8,4,41),NP1,IA,IB,NTEST,TX                        000126
00178     8*          REAL KK,KTAB,KO,NP1                                              000126
00179     9*          INTEGER PROF                                                     000126
00180    10*          DIMENSION BBETAB(7),A1(7),A2(7),A3(7),A4(7)                      000126
00187    11*          DATA BBETAB/0.,.5,.5,1.0,.20.,.50.,.100./,A1/-.68,-.37,.60,3.19,9.13,  000126
00197    12*         X 29.1,105./,A2/-.35,.62,3.15,9.25,22.8,67.1,209./,A3/.55,.71,.99,  000126
00197    13*         X 1.15,1.67,2.76,4.35/,A4/.07,.43,.79,1.30,2.26,4.56,7.09/         000126
00197    14*    C     BAND MODEL PARAMETER PROFILE BY TABULAR INTERPOLATION              000126
00115    15*          DO 1 I=IA,IB                                                     000126
00120    16*          DO 1 L=1,L1                                                      000135
00123    17*          DO 2 J=1,J2                                                      000166
00126    18*          JMIR=J3-J                                                        000166
00126    19*    C     INTERPOLATE FOR KO AND BO, DENORMALIZE KO TO KK,  EQ(14.1)       000166
00127    20*          DO 3 N=2,NK                                                      000175
00132    21*          IF(T(J).GT.TKTAB(    N).AND.N.NE.NK)GO TO 3                      000175
00134    22*          KO(I,L,J)=KTAB(I,L,N-1)+(KTAB(I,L,N)-KTAB(I,L,N-1))              000212
00134    23*         X*(T(J)-TKTAB(    N-1))/(TKTAB(    N)-TKTAB(    N-1))           000212
00135    24*          IF(T(J)..LT.TKTAB(1))KO(I,L,J)=KTAB(I,L,1)                       000224
00137    25*          IF(T(J).GT.TKTAB(NK))KO(I,L,J)=KTAB(I,L,NK)                      000240
00141    26*          GO TO 4                                                          000250
00142    27*        3 CONTINUE                                                         000255
00144    28*        4 KK(I,L,J)=KO(I,L,J)*273.*P(L,J)/T(J)                           000255
00145    29*        2 KK(I,L,JMIR)=KK(I,L,J)                                         000261
00146    30*    C     INTERPOLATE FOR BO                                             000261
00147    31*          DO 1 J=1,J2                                                      000271
00152    32*          DO 5 N=2,NB                                                      000311
00155    33*          IF(T(J).GT.TBTAB(    N).AND.N.NE.NB)GO TO 5                      000311
00157    34*          BO(I,L,J)=BTAB(I,L,N-1)+(BTAB(I,L,N)-BTAB(I,L,N-1))              000326
00157    35*         X*(T(J)-TBTAB(    N-1))/(TBTAB(    N)-TBTAB(    N-1))           000326
00160    36*          IF(T(J)..LT.TBTAB(1))BO(I,L,J)=BTAB(I,L,1)                       000340
00162    37*          IF(T(J).GT.TBTAB(NK))BO(I,L,J)=BTAB(I,L,NK)                      000346
00164    38*          GO TO 1                                                          000354
00165    39*        5 CONTINUE                                                         000376
00167    40*        1 CONTINUE                                                         000376
00167    41*    C     LINE BROADENING AND DENORMALIZE BO TO BR  EQ(14.2)              000376
00173    42*          DO 6 J=1,J2                                                      000376
00176    43*          JMIR=J3-J                                                        000376
00177    44*          DO 6 L=1,L1                                                      000401
00202    45*          DUM=0.                                                           000410
00203    46*          DO 7 LL=1,L2                                                     000412
00206    47*        7 DUM=DUM+ALPH(L,LL)*P(LL,J)                                       000412
00211    48*          DO 6 I=IA,IB                                                     000420
00213    49*          BB(I,L,J)=BO(I,L,J)*DUM                                          000420
00214    50*        6 BB(I,L,JMIR)=BB(I,L,J)                                           000422
00214    51*    C     BE EQ(12)                                                      000422
00220    52*          DO 8 I=IA,IB                                                     000456
00223    53*          DO 8 L=1,L1                                                      000456
00226    54*          BE(I,L,1)=BB(I,L,1)                                              000456
00227    55*          S1=0.                                                            000457
00230    56*          S2=0.                                                            000460
00231    57*          SAV1=KK(I,L,1)*BB(I,L,1)                                         000461
00232    58*          DO 8 J=2,J1                                                      000466
00235    59*          SAV2=KK(I,L,J)*BB(I,L,J)                                         000466
00236    60*          S1=S1+(KK(I,L,J-1)+KK(I,L,J))*DX(J)                              000470
00237    61*          S2=S2+(SAV1+SAV2)*DX(J)                                          000475
00240    62*          SAV1=SAV2                                                        000501
00241    63*          BE(I,L,J)=S2/S1                                                  000503
00242    64*        8 CONTINUE                                                         000523
00242    65*    C     OPTICAL DEPTH U EQ(11), AND ETA EQS(13),(14)                   000523
00246    66*          DO 9 I=IA,IB                                                     000523
00251    67*          DO 9 L=1,L1                                                      000532
00254    68*          ETA(I,L,1)=0.                                                    000537
00255    69*          U(I,L,1)=0.                                                      000540
00256    70*          S1=0.                                                            000541
00257    71*          SAV1=KK(I,L,1)                                                   000542
```

```
00260     72*           DO 9 J=2,J1                                                  000551
00263     73*           BBE=BB(I,L,J)/BF(I,L,J)                                      000551
00264     74*           IF(BBE.GT.100.)BBE=100.                                      000554
00266     75*           SAV2=KK(I,L,J)*BBE**ETA(I,L,J-1)                            000562
00267     76*           S1=S1+(SAV1+SAV2)*DX(J)*.5                                   000572
00270     77*           SAV1=SAV2                                                    000577
00271     78*           U(I,L,J)=S1/BE(I,L,J)                                        000601
00272     79*           DO 10 N=2,7                                                  000606
00275     80*           IF(BBE.GT.BBETAB(N).AND.N.NE.7)GO TO 10                      000606
00277     81*           RATIO=(BBE-BBETAB(N-1))/(BBETAB(N)-BBETAB(N-1))              000623
00300     82*           A5=1.+.185*BBE                                               000631
00301     83*           IF(U(I,L,J).GT.A5)ETA(I,L,J)=(U(I,L,J)+A1(N-1)+(A1(N)-A1(N-1))   000635
00301     84*          X*RATIO)/(U(I,L,J)+(A2(N)-A2(N-1))*RATIO+A2(N-1))             000635
00303     85*           IF(U(I,L,J).LE.A5)ETA(I,L,J)=(U(I,L,J)*(A3(N-1)+(A3(N)-A3(N-1))   000656
00303     86*          X*RATIO))/(A5+U(I,L,J)*((A4(N)-A4(N-1))*RATIO+A4(N-1)))       000656
00305     87*             GO TO 11                                                  000677
00306     88*          10 CONTINUE                                                  000726
00310     89*          11 CONTINUE                                                  000726
00311     90*           9 CONTINUE                                                  000726
00311     91*     C     TAU FOR L1 GASES, EQ (9),(10)                               000726
00315     92*           DO 12 I=IA,IB                                               000726
00320     93*           DO 13 J=1,J1                                                000726
00323     94*           TAU(I,4,J)=1.                                               000726
00324     95*           DO 14 L=1,L1                                                000731
00327     96*           TAU(I,L,J)=EXP(-U(I,L,J)*BE(I,L,J)/SQRT(1.+1.5708*U(I,L,J)))   000731
00336     97*          14 TAU(I,4,J)=TAU(I,4,J)*TAU(I,L,J)                          000751
00332     98*          13 CONTINUE                                                  000766
00334     99*          12 CTAUL(I)=TAU(I,4,J)                                       000766
00334    100*     C     GAS RADIANCE CRL EQ(8)                                      000766
00336    101*           DO 15 I=IA,IB                                               001015
00341    102*           CRL(I)=0.                                                   001017
00342    103*           DO 15 J=2,J1                                                001022
00345    104*           DTAU(I,J)=TAU(I,4,J-1)-TAU(I,4,J)                           001022
00346    105*          15 CRL(I)=CRL(I)+(R(I,J)+R(I,J-1))*DTAU(I,J)*.5/(1.-CTAUL(I))   001024
00351    106*           RETURN                                                      001045
00352    107*           END                                                         001122
```

# APPENDIX G

## WAVES PROGRAM

### Program Symbols

The following FORTRAN symbol list is limited to symbols not in the PROFIL symbol list, APPENDIX D, and not in the NAMELIST data in the section WAVES PROGRAM USE.

| FORTRAN SYMBOL | DESCRIPTION |
|---|---|
| AMAX | Maximum value of dependent profile parameter to determine ZETA |
| AMIN | Minimum value of dependent profile parameter to determine ZETA |
| KEY | Selector for variable profile parameters, KEY=K4+ PROF-1 |
| KEY4 (5) | Index parameter (data statement) |
| K5 | Index parameter to select dependent variable profile parameter |
| NPB | Index parameter NPA-1 |
| PASAV (8,10) | Dependent variable parameter after correction by ZETA |
| PASAVE (4) | Saves initial value of independent variable parameter |
| ZETA (11) | Graph-plotting constant (APPENDIX C) |

# APPENDIX G

# WAVES PROGRAM

```
00101     1*          COMMON PROF,TWB,   L1,J1,J2,J3,C1,PSUM,JM,R1(8),R2(8),X(41),
00101     2*         X PA(4),CTAUL(8),CRL(8),T(41),DX(41),NK,NB,PS,PATH,L2, Y(21),L3,
00101     3*         X CTAU(8,41),R(8,41),CP(6,41),P(6,41),ALPH(3,8),
00101     4*         X TKTAB(    8),KTAB(8,3,8),KO(8,3,21),KK(8,3,41),TBTAB(8),
00101     5*         X BTAB(8,3,8),BO(8,3,21),BB(8,3,41),BE(8,3,41),ETA(8,3,41),
00101     6*         X U(8,3,41),TAU(8,4,41),NP1,IA,IB,NTEST
00103     7*          REAL KK,KTAB,KO,NP1
00104     8*          INTEGER PROF
00105     9*          DIMENSION DPAPA(4),RAB(8),DPA(4),DEL(4),RA(8),DPV(3),PA1(10),
00106    10*         X BOTLIM(4),UPLIM(4),MRL(6),MTAUL(8),G(9,6),GV(9,5),GAS(6),WAVE(8),
00105    11*         X Z(21),RB(8),PASAV(8,10)   ,PASAVE(4),NAME(4),ZETA(11),KEY1(5),
00105    12*         X KEY2(5),KEY3(5),KEY4(5),PW(6),NP(6),PC(6)
00106    13*          REAL MTAUL,MRL,NT,NP,MAX
00107    14*          NAME LIST/NAM1/TREAD,PROF,PATH,I1,WAVE,
00107    15*         X TW,TC,NT,TWB,JP,UPLIM,BOTLIM,L1,L2,PS,PC,NP,PW,NK,
00107    16*         XTKTAB,NB,TBTAB,K4,NPA,PA1,J1,Z,ITER
00110    17*          DATA DEL/4*.01/,NAME/2HNT,4HTC,K,6HPC.ATM,4HTW,K/,J1/21/,Z/0.,.01,
00110    18*         X.02,.05,.1,.2,.3,.4,.5,.7,1.,10*1./,KEY1/2,1,3,0,2/,KEY2/3,3,4,
00110    19*         X 0,3/,KEY3/1,2,1,0,1/,KEY4/2,1,4,0,2/
00121    20*       600 IREAD=0
00122    21*           READ(5,NAM1,END=999)
00125    22*           IF(IREAD.EQ.0)GO TO 111
00127    23*           READ(5,90)(GAS(L),L=1,6)
00132    24*           READ(5,81)((ALPH(L,LL),LL=1,8 ),L=1,L1)
00143    25*           READ(5,81)(((KTAB(I,L,N),N=1,8),I=1,I1),L=1,L1)
00157    26*           READ(5,81)(((BTAB(I,L,N),N=1,8),I=1,I1),L=1,L1)
00173    27*           DO 66 L=1,L1
00176    28*           ALPH(L,L)=1.
00177    29*           DO 66 I=1,I1
00202    30*           DO 68 N=1,NK
00205    31*        68 IF(KTAB(I,L,N).LT. .1E-06)KTAB(I,L,N)=.1E-06
00210    32*           DO 66 N=1,NB
00213    33*        66 IF(BTAB(I,L,N).LT. .1E-06)BTAB(I,L,N)=.1E-06
00220    34*       110 WRITE(6,90)
00222    35*           WRITE(6,NAM1)
00225    36*           WRITE(6,86) (GAS(L),L=1,6)
00230    37*           WRITE(6,87)((ALPH(L,LL),LL=1,8),L=1,L1)
00241    38*           WRITE(6,88)(((KTAB(I,L,N),N=1,8),I=1,I1),L=1,L1)
00255    39*           WRITE(6,89)(((BTAB(I,L,N),N=1,8),I=1,I1),L=1,L1)
00255    40*     C     INITIAL CONDITIONS
00271    41*           IF(K4.EQ.1)PROF=1
00273    42*           IF(K4.EQ.4)PROF=2
00275    43*           KEY=K4+PROF-1
00276    44*           K1=KEY1(KEY)
```

```
00277    45*          42=KEY2(KEY)                                          000374
00300    46*          43=KEY3(KEY)                                          000376
00301    47*          45=KEY4(KEY)                                          000400
00302    48*          NTEST=0                                               000402
00303    49*          IA=1                                                  000403
00304    50*          IB=I1                                                 000405
00305    51*          J3=J1+1                                               000407
00306    52*          J2=(J1+1)/2                                           000411
00307    53*          L3=L1+1                                               000413
00310    54*          C1=PW(1)/PC(1)                                        000415
00311    55*          PA(1)=PT                                              000420
00312    56*          PA(2)=TC                                              000422
00313    57*          PA(3)=PC(1)                                           000424
00314    58*          PA(4)=TW                                              000426
00315    59*          DO 64 K=1,4                                           000455
00320    60*          DPAPA(K)=0.                                           000455
00321    61*          DPA(K)=0.                                             000455
00322    62*          PASAVE(K)=PA(K)                                       000456
00323    63*          DO 64 I=1,6                                           000464
00326    64*          G(K,I)=0.                                             000464
00327    65*          G(K+4,I)=0.                                           000464
00330    66*          G(9,I)=0.                                             000465
00331    67*          PASAV(K,I+4)=0.                                       000466
00332    68*          PASAV(K+4,I+4)=0.                                     000467
00333    69*          DO 64 M=1,41                                          000472
00336    70*          TAU(I+2,K,M)=0.                                       000472
00337    71*          P(I,M)=0.                                             000472
00340    72*          CP(I,M)=0.                                            000473
00341    73*       64 CONTINUE                                              000517
00345    74*          DO 53 I=1,I1                                          000517
00350    75*          R1(I)= .11909E-11 *WAVE(I)**3                         000517
00351    76*       50 R2(I)=1.4388*WAVE(I)                                  000523
00353    77*          DO 51 J=1,J2                                          000532
00356    78*          JMIR=J3-J                                             000532
00357    79*          X(J)=PATH*Z(J)/2.                                     000535
00360    80*          Y(J)=Z(J)                                             000541
00361    81*       51 X(JMIR)=PATH-X(J)                                     000543
00363    82*          DO 59 J=2,J1                                          000553
00366    83*       59 DX(J)=X(J)-X(J-1)                                     000553
00366    84*     C    PRESSURE PROFILE INITIAL PROFILES                     000553
00370    85*          NP1=NP(1)                                             000556
00371    86*          DO 52 J=1,J2                                          000565
00374    87*          DO 53 L=1,L2                                          000605
00377    88*          DUM1=ABS(PC(L)-PW(L))                                 000605
00400    89*          P(L,J)=PC(L)                                          000610
00401    90*          IF(DUM1.EQ.0..OR.J.EQ.J2)GO TO 53                     000612
00403    91*          DUM=1.-Y(J)                                           000617
00404    92*          DUM2=ALOG(DUM1)+ALOG(DUM)/NP(L)                       000621
00405    93*          IF(DUM2.LT. -80.)GO TO 53                             000633
00407    94*       58 P(L,J)=PC(L)-(PC(L)-PW(L))*DUM**(1./NP(L))            000636
00410    95*       53 CONTINUE                                              000656
00412    96*          IF(L1.EQ.1)GO TO 55                                   000656
00412    97*     C    PRESSURE PROFILE RATIO FACTORS CP(L,J)                000656
00414    98*          DO 54 L=2,L1                                          000660
00417    99*       54 CP(L,J)=P(L,J)/P(1,J)                                 000666
00421   100*       55 IF(L2.EQ.L1)GO TO 52                                  000672
00423   101*          DUM=0.                                                000674
```

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00424   102*          DO 56 L=L9,L2                                                    000700
00427   103*       56 DUM=DUM+P(L,J)                                                   000710
00431   104*          DO 57 L=L9,L2                                                    000717
00434   105*       57 CP(L,J)=P(L,J)/DUM                                               000717
00436   106*       52 CONTINUE                                                         000726
00440   107*          CALL TEMP                                                        000726
00441   108*          CALL TRANS                                                       000730
00442   109*          DO 63 I=1,I1                                                     000732
00445   110*          MRL(I)=CRL(I)                                                    000740
00446   111*       63 MTAUL(I)=CTAUL(I)                                                000741
00450   112*          WRITE(6,351)(GAS(L),L=1,6),(K(J),T(J),(P(I,J),I=1,6),J=1,J1)     000744
00464   113*          WRITE(6,90)                                                      000770
00466   114*          WRITE(6,91)                                                      000775
00466   115*    C     INDEPENDENT VARIABLE PARAMETER PA(K4)                            000776
00470   116*          DO 602 I=1,I1                                                    001005
00473   117*          IA=I                                                             001021
00474   118*          IB=I                                                             001023
00475   119*          DO 602 IPA=1,NPA                                                 001030
00500   120*          PA(K4)=PA1(IPA)                                                  001030
00501   121*          ITER1=0                                                          001032
00502   122*          I2=I+1                                                           001033
00502   123*    C     BEGIN ITERATION LOOP                                             001033
00503   124*      700 CALL TEMP                                                        001036
00504   125*          CALL TRANS                                                       001037
00505   126*          IF(NTEST.EQ.1)WRITE(6,75)                                        001041
00510   127*          NTEST=0                                                          001051
00510   128*    C     FIND RESIDUALS, TEST FOR SOLUTION OR MAXIMUM ITERATION NUMBER    001051
00511   129*          TAUAB=CTAUL(I)                                                   001052
00512   130*          RA(I)=CRL(I)                                                     001054
00513   131*          G(I,5)=CRL(I)/MRL(I)-1.                                          001056
00514   132*          S(I2,5)=(MTAUL(I)-CTAUL(I))/(1.-MTAUL(I))                        001061
00515   133*          RESID=SQRT((CRL(I)/MRL(I)-1.)**2+((MTAUL(I)-CTAUL(I))/(1.-MTAUL(I)) 001065
00515   134*         X )**2)                                                           001065
00516   135*          IF((ITER1.GT.0).AND.(ITER1.EQ.ITER.OR.RESID.LT..0001))GO TO 604  001075
00520   136*          ITER1=ITER1+1                                                    001126
00520   137*    C     DERIVATIVES EQ(R11   B12)                                        001126
00521   138*          DEL(I)=.01/PA(I)                                                 001131
00522   139*          DO 3 K=K1,K2,K3                                                  001153
00525   140*          PA(K)=PA(K)*(1.+DEL(K))                                          001153
00526   141*          CALL TEMP                                                        001156
00527   142*          CALL TRANS                                                       001160
00530   143*          RA(I)=CRL(I)                                                     001162
00531   144*          TAUA=CTAUL(I)                                                    001164
00532   145*          PA(K)=PA(K)*(1.-DEL(K))/(1.+DEL(K))                              001166
00533   146*          CALL TEMP                                                        001175
00534   147*          CALL TRANS                                                       001177
00535   148*          RB(I)=CRL(I)                                                     001201
00536   149*          TAUB=CTAUL(I)                                                    001203
00537   150*          PA(K)=PA(K)/(1.-DEL(K))                                          001205
00540   151*          G(I,K)=(RA(I)-RB(I))/(DEL(K)*MRL(I)*2.)                          001212
00541   152*          S(I2,K)=(TAUB-TAUA)/(DEL(K)*(1.-MTAUL(I))*2.)                    001220
00542   153*        3 CONTINUE                                                         001227
00544   154*          CALL TEMP                                                        001227
00545   155*          CALL TRANS                                                       001231
00545   156*    C     CHANGE DERIVATIVE VARIABLES TO CONDENSE ARRAY K=K1,K2,K3 TO K=1,KV 001231
00546   157*          KV=0                                                             001233
00547   158*          DO 7 K=K1,K2,K3                                                  001240
```

```
00552   1590          4V=KV+1                                                  001240
00553   1600          DO 7 IX=I,I2                                             001242
00554   1610        7 GV(IX,KV)=G(IX,K)                                        001250
00555   1620    C     SOLVE FOR PARAMETER FRACTIONAL INCREMENTS WITH DETERMINANT 001250
00561   1630          DENOM=GV(I,1)*GV(I2,2)-GV(I,2)*GV(I2,1)                  001256
00562   1640          DPV(1)=(-G(I,5)*GV(I2,2)+GV(I,2)*G (I2,5))/DENOM         001264
00563   1650          DPV(2)=(-GV(I,1)*G (I2,5)+G(I,5)*GV(I2,1))/DENOM         001273
00563   1660    C     EXPAND INDEX TO ORIGINAL PARAMETER INDEX K=K1,K2,K3      001273
00564   1670          4V=0                                                     001302
00565   1680          DO 20 K=K1,K2,K3                                         001311
00570   1690          4V=KV+1                                                  001311
00571   1700          DPAPA(K)=DPV(KV)                                         001313
00572   1710       20 DPA(K)= DPAPA(K)*PA(K)                                   001316
00572   1720    C     PROPORTIONALLY REDUCE PARAMETER STEP SIZE IF LARGEST STEP EXCEEDS 001316
00572   1730    C    .1*PA(2) OR PA(4), AND .1 FOR PA(1) OR PA(3)              001316
00574   1740          MAX=0.                                                   001321
00575   1750          DO 21 K=K1,K2,K3                                         001325
00600   1760          DUM=ABS(DPAPA(K))                                        001325
00601   1770          IF(K.EQ.1)DUM=ABS(DPA(1))                                001327
00603   1780          IF(K.EQ.3)DUM=ABS(DPA(3))                                001334
00605   1790       21 IF(DUM.GT.MAX)MAX=DUM                                    001341
00610   1800          IF(MAX.LT..1)MAX=.1                                      001351
00612   1810          DO 22 K=K1,K2,K3                                         001365
00615   1820       22 PA (K)=PA(K)+DPA(K)*.1/MAX                               001365
00615   1830    C     TEST FOR PARAMETER  OUTSIDE LIMIT                        001365
00617   1840          DO 23 K=1,4                                              001375
00622   1850          IF(PA (K).GE.BOTLIM(K))GO TO 24                          001375
00624   1860          GO TO 605                                                001401
00625   1870       24 IF(PA (K).LE.UPLIM(K))GO TO 23                           001403
00627   1880          GO TO 605                                                001406
00630   1890       23 CONTINUE                                                 001411
00632   1900          GO TO 700                                                001411
00633   1910      605 WRITE(6,84) NAME(K)                                      001413
00636   1920      604 WRITE(6,821(PA(K),K=1,4),WAVE(I),ITER1,RESID             001423
00644   1930          PASAV(I ,IPA)=PA(K5)                                     001436
00645   1940          PSUM=0.                                                  001440
00646   1950          DO 69 L=1,L1                                             001452
00651   1960       69 PSUM=PSUM+P(L,J2)                                        001452
00653   1970          IF(PSUM.GT.PS1WRITE(6,73)                                001455
00656   1980      602 CONTINUE                                                 001473
00656   1990    C     MAX AND MIN OF DEPENDENT PARAMETER TO DETERMINE ZETA     001473
00661   2000          NPB=NPA-1                                                001473
00662   2010          DO 800 IPA=1,NPA,NPB                                     001475
00665   2020          AMIN=.1E36                                               001512
00666   2030          AMAX=0.                                                  001513
00667   2040          DO 801 I=1,I1                                            001516
00672   2050          IF(PASAV(I,IPA)  .LT.AMIN)AMIN=PASAV(I,IPA)              001516
00674   2060      801 IF(PASAV(I,IPA)  .GT.AMAX)AMAX=PASAV(I,IPA)              001523
00677   2070      800 ZETA(IPA)=(AMIN+AMAX)*.5                                 001533
00701   2080          ZETA(11)=(ZETA(1)-ZETA(NPA))/(PA(NPA)-PA(1))             001541
00702   2090          DO 802 I=1,I1                                            001555
00705   2100          DO 802 IPA=1,NPA                                         001555
00713   2110      802 PASAV(I,IPA)=PASAV(I,IPA)+ZETA(11)*(PA(IPA)-PASAVE(K4))  001555
00713   2120          WRITE(6,803)NAME(K5),ZETA(11),NAME(K4),(PA(J),J=1,10),   001566
00713   2130         X  (WAVE(I),(PASAV(I,IPA),IPA=1,13),I=1,I1)               001566
00731   2140          GO TO  600                                               001617
00732   2150       70 FORMAT (52H ABSORBING GAS PRESSURE GREATER THAN STATIC PRESSURE  ) 001621
00733   2160       80 FORMAT(6A6)                                              001621
00734   2170       81 FORMAT ( 8F6.0)                                          001621
00735   2180       82 FORMAT(1H0,14HPARAMETERS  PA,F9.5,F9.2,F9.5,F9.2,F9.0,7X,I2,9X, 001621
00735   2190         X E7.3)                                                   001621
00736   2200       84 FORMAT(1H0,9HPARAMETER,2X,A6,15H  OUTSIDE LIMIT  )       001621
00737   2210       86 FORMAT(1H0,5H GAS= , 6(4X,A6))                           001621
00740   2220       87 FORMAT(1H0,5HALPH= ,8F10.2/(6X,8F10.2))                  001621
00741   2230       88 FORMAT(1H0,5HKTAB= ,8F10.4/(6X,8F10.4))                  001621
00742   2240       89 FORMAT(1H0,5HBTAB= ,8F10.3/(6X,8F10.3))                  001621
00743   2250       90 FORMAT(1H1)                                              001621
00744   2260       91 FORMAT(1H1,7X,7HPROFILE,5X,4HTEMP,4X,5HAXIAL,4X,5HAXIAL,5X,4HWALL, 001621
00744   2270         X /5X,10HPARAMETERS,3X,8HEXPONENT,3X,4HTEMP,4X,5HPRESS,5X,4HTEMP, 001621
00744   2280         X 2X,10HWAVENUMBER ,5X,4HLAST,8X,3HRMS / 21X,2HNT,6X,4HTC,K,4X, 001621
00744   2290         X 6HPC,ATM,4X,4HTW,K,4X,6H(1/CM),3X,9HITERATION,5X,8HRESIDUAL ) 001621
00745   2300      351 FORMAT(1H0,19HTEMPERATURE PROFILE, 5X,38HPARTIAL PRESSURE PROFILES 001621
00745   2310         X EACH GAS,ATM  /4X,4HX,CM,4X,6HTEMP,K ,6(3X,1A6)//(11X,F7.2,F10.2 001621
00745   2320         X,6F9.4/11X))                                             001621
00746   2330      803 FORMAT(1H0,19X,21HDEPENDENT PARAMETER  ,A5,  13H   WITH ZETA=, 001621
00746   2340         X E8.2/1H0,3X,A6,1X,13F13.3/11H WAVENUMBER /3X,6H(1/CM)/(1X,F6.0 001621
00746   2350         X,4X,10F10.3/))                                           001621
00747   2360      999 STOP                                                     001621
00750   2370          END                                                      001624
```

## APPENDIX B

## EXAMPLE OF PROFILE PROGRAM DATA CARDS AND OUTPUT IN MODE = 1

### Data Cards With Data For Five Wave Numbers (II = 5),

### Profile PROF = 2, Gases $H_2O$ and $N_2$

```
$NAM1 MODE=1,PROF=2,IREAD=1,PATH=100.,II=5,WAVE=1500.,3100.,3600.,
4130.,3333.,303.,
          ERRV=1,ERRH=5,TW=1700.,TC=2000.,NT=.5D,TWB=5.,JB=1
UPLIM=1.,3000.,1.,3000.,.807L2=E.02,600.,.02,993.,LI=1,L2=2,PS=1.
PC=.35,.65,993.,NP=.5,.5,400.,PW=.3,.7,993.,NH=5,TWTAB=600.,1000.,
1400.,2000.,2630.,3000.,.5,.5,.4836,.7878=600.,1000.,1530.,2000.,2580.,
3000.,.0,.2,ITER=10 $
  H2O  N2
   1.   .2
 .268  .438  .393  .318  .288  .268
.0048 .0137 .2372 .0869  .133  .129
.0540  .214  .309  .329  .307  .308
.2386 .2211 .2395 .0635 .0510 .0710
.0033 .0079 .0203 .0463 .0782 .0885
 .107  .145  .309  .693  1.36  2.89
 .099  .113  .236  .663  2.68  10.0
 .144  .182  .320  .683  1.54  3.20
 .113  .157  .345  .783  1.68  3.21
 .075  .394  .187  .483  2.07  16.3
```

### Printout of Input Data

```
$NAM1
MODE    =                 *1
PROF    =                 *2
IREAD   =                 *1
PATH    =     .10000000E+03
II      =                 *5
WAVL    =     .35003003E+34,    .31000000E+04,    .34030030E+34,    .41000333E+04,
              .30003003E+34,    .00000000E+00,    .00330033E+00,    .00000000E+00
HRL     =     .33333333E+33,    .33333333E+33,    .03333333E+30,    .03333333E+00,
              .00000000E+00,    .00000000E+00,    .00033333E+00,    .00000000E+00
HTAUL   =     .33333333E+30,    .00000000E+00,    .00033333E+30,    .00000000E+00,
              .00003333E+30,    .00000000E+00,    .00033333E+30,    .00003333E+00
ERRV    =     .10000300E+01
ERRH    =     .53333F3E+31
TW      =     .17003003E+34
TC      =     .20003000E+04
NT      =     .53333C3E+33
TWB     =     .00003000E+30
JB      =                 *1
UPLIM   =     .13333003E+31,    .33333333E+34,    .13333333E+31,    .30000007E+04
BOTLIM  =     .20003000E-31,    .60000000E+03,    .20033033E-31,    .60000000E+03
L1      =                 *1
L2      =                 *2
PS      =     .10003000E+31
PC      =     .35003003E+00,    .65000000E+00,    .00033333E+00,    .00303033E+00,
              .33333F3E+33,    .33333333E+33
NP      =     .60003003E+30,    .40000000E+00,    .00033333E+30,    .00000000E+00,
              .00003C3E+30,    .00000000E+00
PW      =     .33333C3E+33,    .73033003E+33,    .00333333E+30,    .03333333E+00,
              .00003C3E+00,    .00000000E+00
NH      =                 *5
TWTAB   =     .60033003E+33,    .10000000E+04,    .15033333E+34,    .20333333E+04,
              .25003003E+34,    .30000000E+04,    .00333333E+30,    .00000000E+00
NB      =                 *5
TBTAB   =     .60000003E+33,    .10000000E+04,    .15000333E+04,    .20003333E+04,
              .25033333E+34,    .30000000E+04,    .00333333E+00,    .00303033E+00
JI      =                *21
Z       =     .00000C3E+30,    .10000000E-01,    .20033033E-01,    .60000000E-01,
              .10003003E+30,    .20000000E+00,    .30033033E+00,    .40000000E+00,
              .53333333E+33,    .73033003E+33,    .13333333E+31,    .13333333E+01,
              .10033003E+01,    .10000000E+01,    .10033333E+31,    .10000000E+01,
              .10003333E+31,    .10000000E+01,    .10033333E+31,    .10000000E+01,
              .10003333E+31
ITER    =                *10
TX      =     .3333330C3E+30

$END
```

| GAS= | H2O | N2 | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ALPH= | 1.00 | .20 | .00 | .33 | .33 | .33 | .33 | .33 |
| HTAB= | .2560 | .4380 | .3930 | .3150 | .2880 | .2650 | .0000 | .0000 |
| | .0048 | .0137 | .3372 | .3864 | .1333 | .1293 | .3333 | .3333 |
| | .3540 | .2140 | .3090 | .3290 | .3570 | .3080 | .0000 | .0000 |
| | .2386 | .0211 | .0395 | .0503 | .3610 | .0710 | .0000 | .0000 |
| | .3333 | .0370 | .3203 | .0460 | .0782 | .0885 | .0000 | .0000 |
| BTAB= | .107 | .145 | .309 | .690 | 1.360 | 2.890 | .000 | .333 |
| | .099 | .113 | .236 | .550 | 2.650 | 10.000 | .000 | .300 |
| | .144 | .182 | .320 | .683 | 1.543 | 3.233 | .000 | .000 |
| | .113 | .157 | .345 | .780 | 1.650 | 5.210 | .000 | .000 |
| | .075 | .394 | .187 | .480 | 2.070 | 16.300 | .003 | .300 |

**Profiles and Computation**

| PROFILE PARAMETERS | TEMP EXPONENT NT | AXIAL TEMP TC,K | AXIAL PRESS PC,ATM | WALL TEMP Tw,K | | WALL PRESS PW,ATM | PRESS EXPONENT NP |
|---|---|---|---|---|---|---|---|
| | .50000 | 2000.00 | .35000 | 1700.00 | | .30000 | .80000 |
| PARAMETER ERROR PERCENT | .0% | -1.4% | .6% | 4.5% | WAVENUMBER(1/CM) 3600. | RESIDUAL,PERCENT | 2.0% |
| | .0 | 3.6 | -1.1 | -6.9 | 3100. | | 3.2 |
| | .0 | -.0 | 7.0 | -.2 | 3500. | | 4.4 |
| | .0 | .0 | .0 | .0 | 0. | | .0 |
| | .0 | .0 | .0 | .0 | 0. | | .0 |
| RMS TOTAL | .0 | 4.0 | 7.1 | 8.2 | 0. | | .0 |
| PARAMETER ERROR PERCENT | .0% | -9.7% | 2.9% | 19.4% | WAVENUMBER(1/CM) 3500. | RESIDUAL,PERCENT | 2.0% |
| | .0 | 10.7 | -3.1 | -19.4 | 3400. | | 2.3 |
| | .0 | .0 | 7.0 | .0 | 3500. | | 4.4 |
| | .0 | .0 | .0 | .0 | 0. | | .0 |
| | .0 | .0 | .0 | .0 | 0. | | .0 |
| RMS TOTAL | .0 | 14.4 | 8.2 | 27.4 | 0. | | .0 |
| PARAMETER ERROR PERCENT | .0% | -2.2% | .8% | 5.9% | WAVENUMBER(1/CM) 3500. | RESIDUAL,PERCENT | 2.0% |
| | .0 | 4.6 | -1.3 | -8.4 | 4133. | | 3.6 |
| | .0 | -.1 | 7.0 | .3 | 3500. | | 4.4 |
| | .0 | .0 | .0 | .0 | 0. | | .0 |
| | .0 | .0 | .0 | .0 | 0. | | .0 |
| RMS TOTAL | .0 | 5.2 | 7.2 | 10.3 | 0. | | .0 |
| PARAMETER ERROR PERCENT | .0% | -1.4% | .5% | 4.4% | WAVENUMBER(1/CM) 3500. | RESIDUAL,PERCENT | 2.0% |
| | .0 | 4.8 | -1.4 | -8.6 | 3000. | | 4.3 |
| | .0 | -.1 | 7.0 | .2 | 3500. | | 4.4 |
| | .0 | .0 | .0 | .0 | 0. | | .0 |
| | .0 | .0 | .0 | .0 | 0. | | .0 |
| RMS TOTAL | .0 | 4.9 | 7.2 | 9.7 | 0. | | .0 |

| WAVENUMBER(1/CM)= | 3533. | 3133. | 3400. | 4133. | 3333. | 0. | 0. | 0. |
|---|---|---|---|---|---|---|---|---|
| TRANSMITTANCE= | .598 | .822 | .602 | .854 | .885 | .000 | .000 | .000 |

TEMPERATURE PROFILE — PARTIAL PRESSURE PROFILES EACH GAS,ATM

| X,CM | TEMP,K | 420 | N2 | | | | |
|---|---|---|---|---|---|---|---|
| .00 | 1700.00 | .3300 | .7000 | .0000 | .0000 | .0300 | .0000 |
| .50 | 1705.97 | .3313 | .6990 | .0333 | .0333 | .0330 | .0333 |
| 1.00 | 1711.88 | .3320 | .6980 | .0000 | .0000 | .0000 | .0000 |
| 2.50 | 1729.25 | .3349 | .6951 | .0333 | .0333 | .0330 | .0333 |
| 5.00 | 1757.30 | .3395 | .6905 | .0000 | .0000 | .0000 | .0000 |
| 10.00 | 1808.33 | .3183 | .6820 | .0000 | .0000 | .0000 | .0000 |
| 15.00 | 1853.30 | .3255 | .6745 | .0000 | .0000 | .0000 | .0000 |
| 20.00 | 1892.33 | .3320 | .6680 | .0000 | .0000 | .0000 | .0000 |
| 25.00 | 1925.00 | .3375 | .6625 | .0000 | .0000 | .0000 | .0000 |
| 35.00 | 1973.30 | .3455 | .6545 | .0000 | .0000 | .0000 | .0000 |
| 50.00 | 2000.00 | .3500 | .6500 | .0000 | .0000 | .0000 | .0000 |
| 65.00 | 1973.33 | .3455 | .6545 | .0333 | .0333 | .0000 | .0000 |
| 75.00 | 1925.30 | .3375 | .6625 | .0000 | .0000 | .0300 | .0000 |
| 80.00 | 1892.33 | .3320 | .6680 | .0000 | .0000 | .0000 | .0000 |
| 85.00 | 1853.00 | .3255 | .6745 | .0000 | .0000 | .0000 | .0000 |
| 90.00 | 1808.00 | .3183 | .6820 | .0000 | .0000 | .0000 | .0000 |
| 95.00 | 1757.30 | .3395 | .6905 | .0333 | .0333 | .0330 | .0333 |
| 97.50 | 1729.25 | .3349 | .6951 | .0000 | .0000 | .0000 | .0000 |
| 99.00 | 1711.88 | .3323 | .6980 | .0333 | .0333 | .0330 | .0333 |
| 99.50 | 1705.97 | .3313 | .6990 | .0000 | .0000 | .0000 | .0000 |
| 100.00 | 1700.33 | .3333 | .7000 | .0000 | .0000 | .0000 | .0000 |

## APPENDIX I

### EXAMPLE OF PROFILE PROGRAM DATA CARDS AND OUTPUT IN MODE = 3

Data Cards Continued From Cards of APPENDIX H, With Data For

Four Wave Numbers (I1 =4), Profile PROF = 2

```
$NAM1 MODE=3,I1=4  $
$NAM1 PW=.36,.64,4*0.  $
```

Printout of Input Data

```
$NAM1
MODE     =                 .3
PROF     =                 .2
IREAD    =                 .0
PATH     =     .100000000E+03
I1       =                 .4
WAVE     =     .350000000E+04,   .310000000E+04,   .340000000E+04,   .410000000E+04,
               .300000000E+04,   .000000000E+00,   .000000000E+00,   .000000000E+00
HRL      =     .376097246E-02,   .377280096E-02,   .375668746E-02,   .387192756E-02,
               .373320376E-02,   .000000000E+00,   .000000000E+00,   .000000000E+00
MTAUL    =     .598313286E+00,   .822386571E+00,   .602398856E+00,   .853619336E+00,
               .884803386E+00,   .000000000E+00,   .000000000E+00,   .000000000E+00
ERRV     =     .100000000E+01
ERRK     =     .500000000E+01
TW       =     .170000000E+04
TC       =     .200000000E+04
NT       =     .500000000E+00
TWB      =     .300000000E+03
JB       =                 .1
UPLIM    =     .100000000E+01,   .100000000E+04,   .100000000E+01,   .300000000E+04
BOTLIM   =     .200000000E-01,   .600000000E+03,   .200000000E-01,   .600000000E+03
L1       =                 .1
L2       =                 .2
PS       =     .100000000E+01
PC       =     .350000000E+00,   .650000000E+00,   .000000000E+00,   .000000000E+00,
               .000000000E+00,   .000000000E+00
NP       =     .500000000E+03,   .500000000E+03,   .000000000E+00,   .000000000E+00,
               .000000000E+00,   .000000000E+00
PW       =     .300000000E+00,   .700000000E+00,   .000000000E+00,   .000000000E+00,
               .000000000E+00,   .000000000E+00
NK       =                 .6
TKTAR    =     .600000000E+03,   .100000000E+04,   .150000000E+04,   .200000000E+04,
               .250000000E+04,   .300000000E+04,   .000000000E+00,   .000000000E+00
NB       =                 .6
TBTAR    =     .600000000E+03,   .100000000E+04,   .150000000E+04,   .200000000E+04,
               .250000000E+04,   .300000000E+04,   .000000000E+00,   .000000000E+00
JI       =                <21
Z        =     .000000000E+00,   .100000000E-01,   .200000000E-01,   .500000000E-01,
               .100000000E+00,   .200000000E+00,   .300000000E+00,   .400000000E+00,
               .500000000E+00,   .700000000E+00,   .100000000E+01,   .100000000E+01,
               .100000000E+01,   .100000000E+01,   .100000000E+01,   .100000000E+01,
               .100000000E+01,   .100000000E+01,   .100000000E+01,   .100000000E+01,
               .100000000E+01
ITER     =                 .10
TX       =     .000000000E+00

$END
```

```
$NAMI
MODE    =                 +2
PROF    =                 +2
IREAD   =                 +5
PATH    =  .10000000E+03
II      =                 +4
WAVE    =  .35000000E+34,  .31000000E+04,  .34000000E+34,  .41000000E+04,
           .30000000E+34,  .00000000E+00,  .00000000E+00,  .00000000E+00
HRL     =  .37539724E-32,  .37720859E-32,  .37516874E-32,  .36719278E-32,
MTAUL   =  .59831328E+00,  .82238571E+00,  .60209886E+00,  .85364933E+00,
           .88480338E+00,  .00000000E+00,  .00000000E+00,  .00000000E+00
ERRV    =  .10000000E+01
ERRA    =  .50000000E+31
TM      =  .17000000E+34
TC      =  .20000000E+34
NT      =  .50000000E+00
TWB     =  .00000000E+00
JB      =                 +1
UPLIM   =  .13333333E+31,  .30000000E+34,  .10333333E+31,  .30000000E+04
BOTLIM  =  .20000000E-31,  .60000000E+03,  .20333333E-31,  .60000000E+03
L1      =                 +1
L2      =                 +2
PS      =  .10000000E+31
PC      =  .38000000E+00,  .65000000E+00,  .00000000E+00,  .00000000E+00,
           .33333333E+33,  .70000000E+33
NP      =  .50000000E+00,  .50000000E+00,  .00000000E+00,  .00000000E+00,
           .00000000E+00,  .00000000E+00
PW      =  .36333333E+33,  .64000000E+33,  .00333333E+00,  .33333333E+33,
           .00000000E+00,  .00000000E+00
NK      =                 +6
TKTAR   =  .60000000E+33,  .10000000E+04,  .15000000E+34,  .20000000E+04,
           .25000000E+34,  .30000000E+04,  .00000000E+00,  .00000000E+00
NB      =                 +6
TBTAR   =  .60000000E+33,  .10000000E+04,  .15000000E+04,  .20000000E+04,
           .25000000E+34,  .30000000E+04,  .00000000E+00,  .00000000E+00
JI      =                +21
Z       =  .00000000E+00,  .10000000E-01,  .20000000E-01,  .50000000E-01,
           .10000000E+00,  .20000000E+00,  .30000000E+00,  .40000000E+00,
           .50000000E+33,  .70000000E+33,  .13333333E+31,  .13333333E+31,
           .10000000E+01,  .10000000E+01,  .10000000E+01,  .10000000E+01,
           .13333333E+31,  .10000000E+01,  .10000000E+01,  .10000000E+01,
           .10000000E+31
ITER    =                +10
TK      =  .33333333E+33

$END
```

**Computation and Profiles**

| PROFILE PARAMETERS | TEMP EXPONENT NT | AXIAL TEMP TC,K | AXIAL PRESS PC,ATM | WALL TEMP Tw,K | WALL PRESS PW,ATM | PRESS EXPONENT NP |
|---|---|---|---|---|---|---|
| | .61000 | 2000.00 | .35000 | 1700.00 | .36000 | .60000 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| INCREMENTS DPA | .00000 | .00 | .00000 | .00 | ITERATION= 0 | RMS RESIDUAL= .399-01 | STEP= .000 | | | |
| PARAMETERS PA | .61000 | 2000.00 | .35000 | 1700.00 | RESIDUALS= | -.111-01 | -.749-02 | -.105-01 | -.892-02 | .349-01 |
| | | | | | WAVENUMBER(1/CM)= | 3500. | 3100. | 3400. | 4100. | 3500. |
| INCREMENTS DPA | .00000 | 3.10 | -.01824 | 10.42 | ITERATION= 1 | RMS RESIDUAL= .160-02 | STEP= .129-01 | | | |
| PARAMETERS PA | .61000 | 2033.12 | .33176 | 1710.42 | RESIDUALS= | -.629-03 | .442-04 | -.631-03 | .620-03 | .117-02 |
| | | | | | WAVENUMBER(1/CM)= | 3500. | 3100. | 3400. | 4100. | 3500. |
| INCREMENTS DPA | .00000 | -1.61 | -.00053 | 3.49 | ITERATION= 2 | RMS RESIDUAL= .626-03 | STEP= .311-02 | | | |
| PARAMETERS PA | .61000 | 2031.29 | .33122 | 1713.91 | RESIDUALS= | -.410-05 | -.372-03 | -.228-03 | .445-03 | -.599-04 |
| | | | | | WAVENUMBER(1/CM)= | 3500. | 3100. | 3400. | 4100. | 3500. |
| INCREMENTS DPA | .00000 | -.05 | .00003 | .13 | ITERATION= 3 | RMS RESIDUAL= .623-03 | STEP= .113-03 | | | |
| PARAMETERS PA | .61000 | 2031.23 | .33125 | 1714.03 | RESIDUALS= | .280-04 | -.375-03 | -.204-03 | .453-03 | -.709-05 |
| | | | | | WAVENUMBER(1/CM)= | 3500. | 3100. | 3400. | 4100. | 3500. |
| INCREMENTS DPA | .00000 | .00 | .00000 | .00 | ITERATION= 4 | RMS RESIDUAL= .623-03 | STEP= .929-06 | | | |
| PARAMETERS PA | .61000 | 2031.23 | .33126 | 1714.04 | RESIDUALS= | .287-04 | -.375-03 | -.203-03 | .453-03 | -.521-05 |
| | | | | | WAVENUMBER(1/CM)= | 3500. | 3100. | 3400. | 4100. | 3500. |

| PARAMETER ERROR PERCENT | | | | | WAVENUMBER(1/CM) | RESIDUAL,PERCENT |
|---|---|---|---|---|---|---|
| | .0% | -1.3% | .4% | 3.2% | 3500. | 9.0% |
| | .0 | 2.6 | -.7 | -4.5 | 3100. | 3.2 |
| | .0 | -.7 | .2 | 1.9 | 3400. | 2.0 |
| | .0 | 1.9 | -.4 | -3.0 | 4100. | 3.6 |
| | .0 | -.1 | 7.1 | .2 | 3500. | 4.4 |
| RMS TOTAL | .0 | 3.5 | 7.1 | 6.6 | 0. | .0 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| WAVENUMBER(1/CM)= | 3500. | 3100. | 3400. | 4100. | 3333. | 3. | 3. | 3. |
| TRANSMITTANCE= | .598 | .822 | .602 | .853 | .000 | .000 | .000 | .000 |

| TEMPERATURE PROFILE | | PARTIAL PRESSURE PROFILES EACH GAS,ATM | | | | | |
|---|---|---|---|---|---|---|---|
| X,CM | TEMP,K | H2O | N2 | | | | |
| .33 | 1714.34 | .3437 | .6593 | .0000 | .0000 | .0000 | .0000 |
| .50 | 1719.75 | .3405 | .6595 | .0000 | .0000 | .0000 | .0000 |
| 1.00 | 1726.41 | .3403 | .6597 | .0000 | .0000 | .0000 | .0000 |
| 2.50 | 1742.04 | .3398 | .6602 | .0000 | .0000 | .0000 | .0000 |
| 5.00 | 1768.60 | .3389 | .6611 | .0000 | .0000 | .0000 | .0000 |
| 10.00 | 1817.43 | .3373 | .6627 | .0000 | .0000 | .0000 | .0000 |
| 15.00 | 1863.51 | .3359 | .6641 | .0000 | .0000 | .0000 | .0000 |
| 20.00 | 1897.84 | .3347 | .6653 | .0000 | .0000 | .0000 | .0000 |
| 25.00 | 1929.43 | .3336 | .6664 | .0000 | .0000 | .0000 | .0000 |
| 35.00 | 1975.38 | .3321 | .6679 | .0000 | .0000 | .0000 | .0000 |
| 50.00 | 2001.23 | .3313 | .6687 | .0000 | .0000 | .0000 | .0000 |
| 65.00 | 1975.38 | .3321 | .6679 | .0000 | .0000 | .0000 | .0000 |
| 75.00 | 1929.43 | .3336 | .6664 | .0000 | .0000 | .0000 | .0000 |
| 80.00 | 1897.84 | .3347 | .6653 | .0000 | .0000 | .0000 | .0000 |
| 85.00 | 1860.51 | .3359 | .6641 | .0000 | .0000 | .0000 | .0000 |
| 90.00 | 1817.43 | .3373 | .6627 | .0000 | .0000 | .0000 | .0000 |
| 95.00 | 1768.60 | .3389 | .6611 | .0000 | .0000 | .0000 | .0000 |
| 97.50 | 1742.04 | .3398 | .6602 | .0000 | .0000 | .0000 | .0000 |
| 99.00 | 1725.41 | .3403 | .6597 | .0000 | .0000 | .0000 | .0000 |
| 99.50 | 1719.75 | .3405 | .6595 | .0000 | .0000 | .0000 | .0000 |
| 100.00 | 1714.34 | .3437 | .6593 | .0000 | .0000 | .0000 | .0000 |

## APPENDIX J

## EXAMPLE OF WAVES PROGRAM DATA CARDS AND OUTPUT

### Data Cards With Data For Four Wave Numbers (II = 4), Gases $H_2O$ and $N_2$

```
$NAM1 PROF=1,IREAD=1,PATH=100.,II=4,WAVE=3100.,3500.,3775.,4100.,400.,
                    TW=1000.,TC=2000.,NT=25,TWB=0.  ,
      JB=1,UPLIM=1.,3500.,2.,3000.,BOTLIM=.72,600.,.02,.02,
   L1=1,L2=2,PS=1.,PC=.35,.65,400.,NP=6.,5,400.,PW=.3,.70,400.,
   NK=6,TKTAB=600., 1000.,1500.,
2000.,2500.,3000.,0.,0.,NA=6,TBTAB=600.,1000.,1500.,2000.,2500.,
3000.,.1,.1,KW=1,NPA=8,PAI=.05,.1,.15,.2,.3,.4,.5,.6,.6,ITER=10 $
  H2O    N2
   1.     .2
.0048  .0137  .0372  .0864   .133   .129
 .258   .438   .393   .315   .288   .265
 .124   .120   .119   .115   .116   .109
.0086  .0211  .0395  .0503  .0610  .0710
 .094   .113   .236   .550  2.450  16.0
 .107   .145   .309   .690  1.36   2.89
 .233   .264   .374   .650  1.41   6.28
 .113   .157   .345   .780  1.85   6.21
```

### Printout of Input Data

```
$NAM1
IREAD  =
PROF   =                    •1
PATH   =                    •1
II     =      •10000000E•03
WAVE   =                    •4
                •31000000E•04,      •35000000E•04,      •37750000E•04,      •41000000E•04,
TW     =        •00000000E•00,      •00000000E•00,      •00000000E•00,      •00000000E•00
TC     =        •13333000E•04
NT     =        •20000000E•04
TWB    =        •25000000E•00
JB     =        •33333000E•00
UPLIM  =                    •1
BOTLIM =      •10000000E•01,      •35000000E•04,      •20000000E•01,      •30000000E•04
L1     =      •20000000E-01,      •60000000E•03,      •20333333E-01,      •23000000E-01
L2     =                    •1
PS     =                    •2
PC     =      •10000000E•01
                •35000000E•00,      •65000000E•00,      •00000000E•00,      •00000000E•00,
NP     =        •33333000E•00,      •00000000E•00
                •50000000E•00,      •50000000E•00,      •00000000E•00,      •00000000E•00,
PW     =        •00000000E•00,      •00000000E•00
                •33333000E•00,      •73000000E•00,      •00000000E•00,      •00000000E•00,
NK     =        •00000000E•00,      •00000000E•00
TKTAB  =                    •6
                •60000000E•03,      •10000000E•04,      •15000000E•04,      •20000000E•04,
NA     =        •25000000E•04,      •30000000E•04,      •00000000E•00,      •00000000E•00
TBTAB  =                    •6
                •60000000E•03,      •10000000E•04,      •15000000E•04,      •20000000E•04,
KW     =        •25000000E•04,      •30000000E•04,      •15000000E•04,      •20000000E•04,
NPA    =                    •1                          •00000000E•00,      •10000000E•00
PAI    =                    •8
                •50000000E-01,      •10000000E•00,      •15000000E•00,      •20000000E•00,
                •33333000E•00,      •43333000E•00,      •53333000E•00,      •63333000E•00,
JI     =        •60000000E•00,      •60000000E•00
Z      =                   •21
                •30000000E•00,      •10000000E-01,      •20000000E-01,      •50000000E-01,
                •10000000E•00,      •20000000E•00,      •30000000E•00,      •40000000E•00,
                •50000000E•00,      •70000000E•00,      •10000000E•01,      •10000000E•01,
                •10000000E•01,      •10000000E•01,      •10000000E•01,      •10000000E•01,
                •10000000E•01,      •10000000E•01,      •10000000E•01,      •10000000E•01,
ITER   =        •10000000E•01
                          •10
$END
```

| GAS= | H2O | N2 | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ALPH2 | 1.00 | .20 | .00 | .00 | .00 | .00 | .00 | .00 |
| KTAB= | .0048 | .0137 | .0372 | .0864 | .1333 | .1293 | .0333 | .0333 |
| | .2580 | .4380 | .3930 | .3150 | .2880 | .2650 | .0000 | .0000 |
| | .1240 | .1200 | .1190 | .1153 | .1150 | .1093 | .0000 | .0000 |
| | .0086 | .0211 | .0395 | .0503 | .0610 | .0710 | .0000 | .0000 |
| BTAB= | .094 | .113 | .236 | .550 | 2.450 | 16.000 | .000 | .000 |
| | .107 | .145 | .309 | .690 | 1.360 | 2.890 | .000 | .000 |
| | .233 | .264 | .374 | .650 | 1.413 | 6.280 | .000 | .000 |
| | .113 | .157 | .345 | .780 | 1.850 | 5.210 | .000 | .000 |

## Profiles and Computation

| TEMPERATURE PROFILE X,CM | TEMP,° | PARTIAL PRESSURE PROFILES EACH GAS,ATM H2O | N2 | | | | |
|---|---|---|---|---|---|---|---|
| .00 | 1000.00 | .3300 | .7000 | .0000 | .0000 | .0000 | .0000 |
| .50 | 1039.40 | .3313 | .6990 | .0000 | .0000 | .0000 | .0000 |
| 1.00 | 1077.63 | .3320 | .6980 | .0000 | .0000 | .0000 | .0000 |
| 2.50 | 1185.49 | .3349 | .6951 | .0000 | .0000 | .0000 | .0000 |
| 5.00 | 1343.90 | .3395 | .6905 | .0000 | .0000 | .0000 | .0000 |
| 10.00 | 1590.40 | .3180 | .6820 | .0000 | .0000 | .0000 | .0000 |
| 15.00 | 1759.90 | .3255 | .6745 | .0000 | .0000 | .0000 | .0000 |
| 20.00 | 1873.40 | .3320 | .6680 | .0000 | .0000 | .0000 | .0000 |
| 25.00 | 1937.50 | .3375 | .6625 | .0000 | .0000 | .0000 | .0000 |
| 35.00 | 1991.90 | .3455 | .6545 | .0000 | .0000 | .0000 | .0000 |
| 50.00 | 2000.00 | .3500 | .6500 | .0000 | .0000 | .0000 | .0000 |
| 65.00 | 1991.90 | .3455 | .6545 | .0000 | .0000 | .0000 | .0000 |
| 75.00 | 1937.50 | .3375 | .6625 | .0000 | .0000 | .0000 | .0000 |
| 80.00 | 1870.40 | .3320 | .6680 | .0000 | .0000 | .0000 | .0000 |
| 85.00 | 1759.90 | .3255 | .6745 | .0000 | .0000 | .0000 | .0000 |
| 90.00 | 1590.40 | .3180 | .6820 | .0000 | .0000 | .0000 | .0000 |
| 95.00 | 1343.90 | .3395 | .6905 | .0000 | .0000 | .0000 | .0000 |
| 97.50 | 1185.49 | .3349 | .6951 | .0000 | .0000 | .0000 | .0000 |
| 99.00 | 1077.63 | .3320 | .6980 | .0000 | .0000 | .0000 | .0000 |
| 99.50 | 1039.40 | .3313 | .6990 | .0000 | .0000 | .0000 | .0000 |
| 100.00 | 1000.00 | .3300 | .7000 | .0000 | .0000 | .0000 | .0000 |

| PROFILE PARAMETERS | | TEMP EXPONENT NT | AXIAL TEMP TC,K | AXIAL PRESS PC,ATM | WALL TEMP TW,K | WAVENUMBER (1/CM) | LAST ITERATION | RMS RESIDUAL |
|---|---|---|---|---|---|---|---|---|
| PARAMETERS | PA | .05000 | 1934.37 | .33712 | 1000.00 | 3130. | 3 | .996-07 |
| PARAMETERS | PA | .10000 | 1928.85 | .34025 | 1000.00 | 3130. | 2 | .126-06 |
| PARAMETERS | PA | .15000 | 1951.98 | .34395 | 1000.00 | 3130. | 2 | .894-07 |
| PARAMETERS | PA | .20000 | 1976.28 | .34659 | 1000.00 | 3130. | 2 | .996-07 |
| PARAMETERS | PA | .30000 | 2021.18 | .35001 | 1000.00 | 3130. | 3 | .332-04 |
| PARAMETERS | PA | .40000 | 2063.31 | .34800 | 1000.00 | 3130. | 3 | .225-05 |
| PARAMETERS | PA | .60000 | 2135.49 | .34832 | 1000.00 | 3130. | 2 | .767-04 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| PARAMETERS | PA | .63000 | 2144.81 | .34936 | 1000.00 | 3500. | 2 | .437-04 |
| PARAMETERS | PA | .05000 | 1834.74 | .36788 | 1000.00 | 3500. | 3 | .722-05 |
| PARAMETERS | PA | .10000 | 1884.00 | .36068 | 1000.00 | 3500. | 2 | .138-05 |
| PARAMETERS | PA | .15000 | 1925.00 | .35466 | 1000.00 | 3500. | 2 | .251-06 |
| PARAMETERS | PA | .20000 | 1963.77 | .35223 | 1333.30 | 3500. | 2 | .144-06 |
| PARAMETERS | PA | .30000 | 2031.58 | .34620 | 1000.00 | 3500. | 2 | .545-04 |
| PARAMETERS | PA | .40000 | 2091.55 | .34035 | 1000.00 | 3500. | 2 | .722-05 |
| PARAMETERS | PA | .50000 | 2150.02 | .33688 | 1000.00 | 3500. | 2 | .617-05 |
| PARAMETERS | PA | .60000 | 2205.47 | .33533 | 1000.00 | 3500. | 2 | .287-05 |
| PARAMETERS | PA | .05000 | 1839.94 | .36545 | 1333.30 | 3775. | 3 | .271-04 |
| PARAMETERS | PA | .10000 | 1883.20 | .35384 | 1000.00 | 3775. | 2 | .230-06 |
| PARAMETERS | PA | .15000 | 1923.17 | .35244 | 1000.00 | 3775. | 2 | .634-07 |
| PARAMETERS | PA | .20000 | 1962.10 | .35107 | 1000.00 | 3775. | 2 | .684-07 |
| PARAMETERS | PA | .30000 | 2034.16 | .34650 | 1000.00 | 3775. | 2 | .117-04 |
| PARAMETERS | PA | .40000 | 2099.36 | .34027 | 1333.30 | 3775. | 2 | .653-05 |
| PARAMETERS | PA | .50000 | 2162.49 | .33581 | 1000.00 | 3775. | 2 | .278-05 |
| PARAMETERS | PA | .60000 | 2222.74 | .33276 | 1000.00 | 3775. | 2 | .741-06 |
| PARAMETERS | PA | .05000 | 1882.26 | .34533 | 1000.00 | 4100. | 3 | .173-04 |
| PARAMETERS | PA | .10000 | 1912.02 | .34667 | 1000.00 | 4100. | 2 | .689-07 |
| PARAMETERS | PA | .15000 | 1941.17 | .34788 | 1333.30 | 4100. | 2 | .114-06 |
| PARAMETERS | PA | .20000 | 1970.48 | .34898 | 1333.30 | 4100. | 2 | .544-07 |
| PARAMETERS | PA | .30000 | 2028.86 | .34942 | 1000.00 | 4100. | 2 | .508-04 |
| PARAMETERS | PA | .40000 | 2086.02 | .34815 | 1000.00 | 4100. | 2 | .966-06 |
| PARAMETERS | PA | .50000 | 2142.20 | .34760 | 1333.30 | 4100. | 2 | .648-06 |
| PARAMETERS | PA | .60000 | 2196.28 | .34756 | 1000.00 | 4100. | 2 | .420-06 |

DEPENDENT PARAMETER TC,K WITH ZETA= -.57+03

| NT WAVENUMBER (1/CM) | .050 | .100 | .150 | .200 | .300 | .400 | .500 | .600 | .800 | .900 |
|---|---|---|---|---|---|---|---|---|---|---|
| 3100. | 2018.593 | 2014.617 | 2009.089 | 2004.835 | 1992.628 | 1977.652 | 1962.721 | 1944.929 | .000 | .000 |
| 3500. | 1949.232 | 1969.660 | 1982.106 | 1992.329 | 2003.023 | 2005.885 | 2007.253 | 2005.589 | .000 | .000 |
| 3775. | 1954.161 | 1968.863 | 1980.276 | 1990.654 | 2005.611 | 2013.694 | 2019.719 | 2022.863 | .000 | .000 |
| 4100. | 1996.476 | 1997.681 | 1998.276 | 1999.334 | 2003.308 | 2003.361 | 1999.428 | 1996.399 | .000 | .000 |

$FIN

## APPENDIX K

## EXAMPLE OF PROFILE WITH HIGH-TEMPERATURE CORE

### Data Cards With Measured Data, Two Wave Numbers, Profile PROF = 2

### No Boundary Layer, Gases $H_2O$ and $N_2$

```
$NAM1 MODE=2,PROF=2,IREAD=1,PATH=100.,I1=2,WAVE=3500.,3100.,6*0.,
MRL=.007113,.003433,6*0.,MTAUL=.4316,.8352,6*0.,
ERRV=1.,ERRK=5.,TW=1.00.,TC=1850.,NT=.50,TWB=1100.,JB=5,UPLIM=1.,3000.,
1.,7000.,BOTLIM=.02,600.,.02,600.,L1=1,L2=2,PS=1.,PC=.35,.65,4*0.,
NP=2*.5,4*0.,PW=.3,.7,4*0.,NK=6,TKTAB=600.,1000.,1500.,2000.,2500.,
3000.,2*0.,NB=6,TBTAB=600.,1000.,1500.,2000.,2500.,3000.,2*0.,
      J1=25,Z=0.,.01,.02,.05,.1,.2,.3,.4,.5,.6,.7,.8,.9*1.,
ITER=10,TX=600.  $
  H2O   N2
   1.    .2
 .258  .438  .393  .315  .288  .265
.0048 .0137 .0372 .0864  .133  .129
 .326  .525  1.10  2.18  3.35  4.35
 .094  .113  .236  .550  2.45  18.0
```

### Printout of Input Data

```
$NAM1
MODE    =                 *2
PROF    =                 *2
IREAD   =                 *1
PATH    =     .100000000E*02
I1      =                 *2
WAVE    =     .350000000E*04,   .310000000E*04,   .000000000E*00,   .000000000E*00,
              .000000000E*00,   .000000000E*00,   .000000000E*00,   .000000000E*00
MRL     =     .311300000E-02,   .343300000E-02,   .000000000E*00,   .000000000E*00,
              .000000000E*00,   .000000000E*00,   .000000000E*00,   .000000000E*00
MTAUL   =     .431600000E*00,   .835200000E*00,   .000000000E*00,   .000000000E*00,
              .000000000E*00,   .000000000E*00,   .000000000E*00,   .000000000E*00
ERRV    =     .100000000E*01
ERRK    =     .500000000E*01
TW      =     .120000000E*04
TC      =     .185000000E*04
NT      =     .500000000E*00
TWB     =     .110000000E*04
JB      =                 *5
UPLIM   =     .100000000E*01,   .300000000E*04,   .100000000E*01,   .300000000E*04
BOTLIM  =     .200000000E-01,   .600000000E*03,   .200000000E-01,   .600000000E*03
L1      =                 *1
L2      =                 *2
PS      =     .100000000E*01
PC      =     .350000000E*00,   .650000000E*00,   .000000000E*00,   .000000000E*00,
              .000000000E*00,   .000000000E*00
NP      =     .500000000E*00,   .500000000E*00,   .000000000E*00,   .000000000E*00,
              .000000000E*00,   .000000000E*00
PW      =     .300000000E*00,   .700000000E*00,   .000000000E*00,   .000000000E*00,
              .000000000E*00,   .000000000E*00
NK      =                 *6
TKTAB   =     .600000000E*03,   .100000000E*04,   .150000000E*04,   .200000000E*04,
              .250000000E*04,   .300000000E*04,   .000000000E*00,   .000000000E*00
NB      =                 *6
TBTAB   =     .600000000E*03,   .100000000E*04,   .150000000E*04,   .200000000E*04,
              .250000000E*04,   .300000000E*04,   .000000000E*00,   .000000000E*00
J1      =                *25
Z       =     .000000000E*00,   .100000000E-01,   .200000000E-01,   .500000000E-01,
              .100000000E*00,   .200000000E*00,   .300000000E*00,   .400000000E*00,
              .500000000E*00,   .600000000E*00,   .700000000E*00,   .800000000E*00,
              .100000000E*01,   .100000000E*01,   .100000000E*01,   .100000000E*01,
              .100000000E*01,   .100000000E*01,   .100000000E*01,   .100000000E*01,
              .100000000E*01
ITER    =                *10
TX      =     .600000000E*00

$END

 GAS=        H2O        N2

ALPH=       1.00        .20        .00        .00        .00        .00        .00        .00

KTAB=       .2580      .4380      .3930      .3150      .2880      .2650      .0000      .0000
            .0048      .0137      .0372      .0864      .1330      .1290      .0000      .0000
BTAB=       .326       .525      1.100      2.180      3.350      4.350       .000       .000
            .094       .113       .236       .550      2.450     18.000       .000       .000
```

**Computation and Profiles**

| PROFILE PARAMETERS | TEMP EXPONENT NT | AXIAL TEMP TC,K | AXIAL PRESS PC,ATM | WALL TEMP TW,K | WALL PRESS PW,ATM | PRESS EXPONENT NP |
|---|---|---|---|---|---|---|
| | .50030 | 1850.00 | .35000 | 1200.00 | .30000 | .50000 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| INCREMENTS | DPA | .03000 | .00 | .00000 | .00 | ITERATION= 0 | RMS RESIDUAL= .342+00 | STEP= .000 | | | |
| PARAMETERS | PA | .53003 | 1850.00 | .35000 | 1200.00 | RESIDUALS= | -.274+00 | -.204+00 | .165-01 | .000 | .000 |
| | | | | | | WAVENUMBER(1/CM)= | 3500. | 3100. | 3500. | 0. | 0. |
| INCREMENTS | DPA | .03003 | 42.66 | -.00057 | 120.00 | ITERATION= 1 | RMS RESIDUAL= .220+00 | STEP= .123+00 | | | |
| PARAMETERS | PA | .53000 | 1892.66 | .34943 | 1320.00 | RESIDUALS= | -.176+00 | -.132+00 | .102-01 | .000 | .000 |
| | | | | | | WAVENUMBER(1/CM)= | 3500. | 3100. | 3500. | 0. | 0. |
| INCREMENTS | DPA | .03003 | 56.15 | -.00019 | 132.00 | ITERATION= 2 | RMS RESIDUAL= .646-01 | STEP= .130+00 | | | |
| PARAMETERS | PA | .53000 | 1948.81 | .34925 | 1452.00 | RESIDUALS= | -.513-01 | -.392-01 | .231-02 | .000 | .000 |
| | | | | | | WAVENUMBER(1/CM)= | 3500. | 3100. | 3500. | 0. | 0. |
| INCREMENTS | DPA | .03003 | 24.93 | .00066 | 47.19 | ITERATION= 3 | RMS RESIDUAL= .982-03 | STEP= .456-01 | | | |
| PARAMETERS | PA | .53000 | 1973.70 | .34991 | 1499.19 | RESIDUALS= | .747-03 | .636-03 | -.198-03 | .000 | .000 |
| | | | | | | WAVENUMBER(1/CM)= | 3500. | 3100. | 3500. | 0. | 0. |
| INCREMENTS | DPA | .03003 | -.42 | .00010 | -.52 | ITERATION= 4 | RMS RESIDUAL= .992-07 | STEP= .586-03 | | | |
| PARAMETERS | PA | .53000 | 1973.29 | .35000 | 1498.67 | RESIDUALS= | .596-07 | .447-07 | -.655-07 | .000 | .000 |
| | | | | | | WAVENUMBER(1/CM)= | 3500. | 3100. | 3500. | 0. | 0. |

| PARAMETER ERROR PERCENT | | | | | WAVENUMBER(1/CM) | RESIDUAL,PERCENT |
|---|---|---|---|---|---|---|
| | .0% | -.7% | .2% | 3.5% | 3500. | 1.6% |
| | .0 | 2.8 | .0 | -7.0 | 3100. | 3.3 |
| | .0 | -.1 | 6.3 | .6 | 3500. | 3.4 |
| | .0 | .3 | .0 | .0 | 0. | .0 |
| | .0 | .0 | .0 | .0 | 0. | .0 |
| RMS TOTAL | .0 | 2.9 | 6.3 | 7.8 | 0. | .0 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| WAVENUMBER(1/CM)= | 3500. | 3100. | 0. | 0. | 0. | 0. | 0. | 0. |
| TRANSMITTANCE= | .432 | .835 | .000 | .000 | .000 | .000 | .000 | .000 |

TEMPERATURE PROFILE — PARTIAL PRESSURE PROFILES EACH GAS,ATM

| X,CM | TEMP,K | CO2 | N2 | | | | |
|---|---|---|---|---|---|---|---|
| .00 | 1100.00 | .3303 | .7000 | .0000 | .0000 | .0000 | .0000 |
| .50 | 1185.19 | .3313 | .6990 | .0000 | .0000 | .0000 | .0000 |
| 1.00 | 1262.32 | .3323 | .6980 | .0000 | .0000 | .0000 | .0000 |
| 2.50 | 1445.28 | .3349 | .6951 | .0000 | .0000 | .0000 | .0000 |
| 5.00 | 1588.85 | .3395 | .6905 | .0000 | .0000 | .0000 | .0000 |
| 10.00 | 1669.53 | .3180 | .6820 | .0000 | .0000 | .0000 | .0000 |
| 15.00 | 1740.73 | .3255 | .6745 | .0000 | .0000 | .0000 | .0000 |
| 20.00 | 1802.43 | .3320 | .6680 | .0000 | .0000 | .0000 | .0000 |
| 25.00 | 1854.63 | .3375 | .6625 | .0000 | .0000 | .0000 | .0000 |
| 30.00 | 1897.35 | .3420 | .6580 | .0000 | .0000 | .0000 | .0000 |
| 35.00 | 1930.57 | .3455 | .6545 | .0000 | .0000 | .0000 | .0000 |
| 40.00 | 1954.30 | .3480 | .6520 | .0000 | .0000 | .0000 | .0000 |
| 50.00 | 1973.29 | .3500 | .6500 | .0000 | .0000 | .0000 | .0000 |
| 60.00 | 1954.30 | .3480 | .6520 | .0000 | .0000 | .0000 | .0000 |
| 65.00 | 1930.57 | .3455 | .6545 | .0000 | .0000 | .0000 | .0000 |
| 70.00 | 1897.35 | .3420 | .6580 | .0000 | .0000 | .0000 | .0000 |
| 75.00 | 1854.63 | .3375 | .6625 | .0000 | .0000 | .0000 | .0000 |
| 80.00 | 1802.43 | .3320 | .6680 | .0000 | .0000 | .0000 | .0000 |
| 85.00 | 1740.73 | .3255 | .6745 | .0000 | .0000 | .0000 | .0000 |
| 90.00 | 1669.53 | .3180 | .6820 | .0000 | .0000 | .0000 | .0000 |
| 95.00 | 1588.85 | .3395 | .6905 | .0000 | .0000 | .0000 | .0000 |
| 97.50 | 1445.28 | .3349 | .6951 | .0000 | .0000 | .0000 | .0000 |
| 99.00 | 1262.32 | .3323 | .6980 | .0000 | .0000 | .0000 | .0000 |
| 99.50 | 1185.19 | .3313 | .6990 | .0000 | .0000 | .0000 | .0000 |
| 100.00 | 1100.00 | .3303 | .7000 | .0000 | .0000 | .0000 | .0000 |

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TABLE I. - COEFFICIENTS TO BE USED IN EQUATION (16)

| $\beta/\beta_e$ | $A_1$ | $A_2$ | $A_3$ | $A_4$ | $A_5$ |
|---|---|---|---|---|---|
| 0 | -0.68 | -0.35 | 0.55 | 0.07 | 1.00 |
| 2 | -.37 | .62 | .71 | .43 | 1.37 |
| 5 | .60 | 3.15 | .90 | .79 | 1.93 |
| 10 | 3.19 | 9.25 | 1.15 | 1.30 | 2.85 |
| 20 | 9.10 | 22.3 | 1.63 | 2.26 | 4.70 |
| 50 | 29.1 | 67.1 | 2.78 | 4.56 | 10.25 |
| 100 | 105 | 209 | 4.05 | 7.09 | 19.50 |

TABLE II. - SPECTRAL LINE BROADENING COEFFICIENT, $\alpha^*$ (FROM REF. 16)

| Absorbing gas | Broadening gas | | | | | | |
|---|---|---|---|---|---|---|---|
| | $H_2O$ | $CO_2$ | CO | $CH_2$ | $N_2$ | $H_2$ | $O_2$ |
| $H_2O$ | 1 | 0.77 | | | 0.20 | 0.1 | |
| $CO_2$ | | 1 | | | .77 | 1.17 | 0.81 |
| CO | | | 1 | 1.12 | .95 | .85 | |
| $CH_4$ | | 1.25 | | 1 | .75 | | |

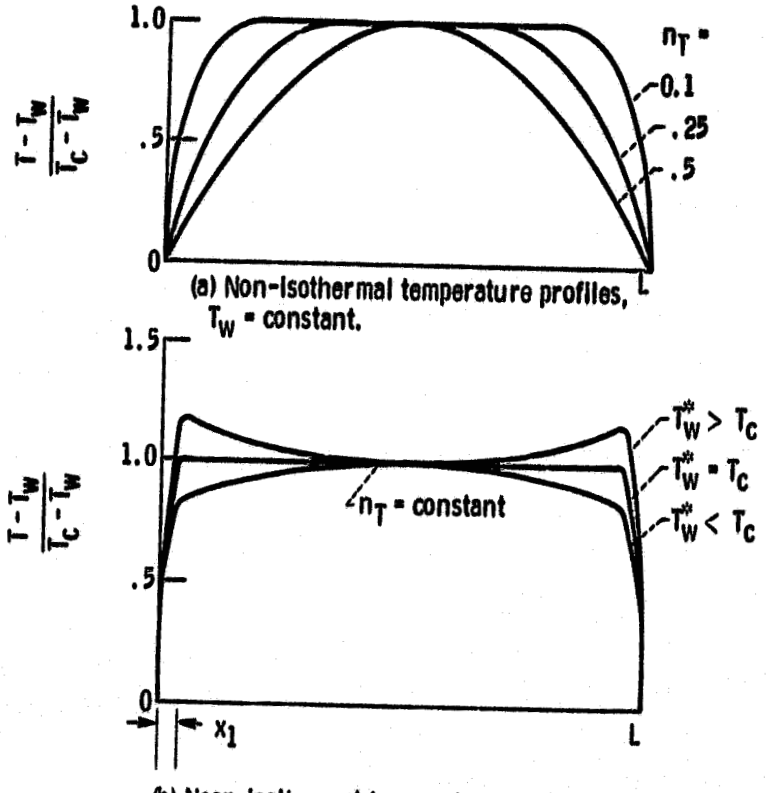
## TABLE III. - ESTIMATED PERCENT ERROR OF $T_c$ AND $T_w^*$ AND TRANSMITTANCE FOR VARIOUS PATH LENGTHS FOR PROFILE OF FIGURE 1(b)

[Measurement wavenumbers 3100, 3400, 3500, and 4100 $cm^{-1}$; $T_c$ = 2000 K, $n_T$ = 0.5, $p_c$ = 0.35 atm, $p_w$ = 0.30 atm, $n_p$ = 0.5. Errors caused by one percent error of radiance measurement, and five percent error of tabulated absorption coefficients.]

| Percent error in $T_c$ | | | | |
|---|---|---|---|---|
| $T_w^*$, K | Path length, cm | | | |
| | 50 | 100 | 200 | 400 |
| 1200 | 3.0 | 2.1 | 1.4 | 1.0 |
| 2000 | 11.5 | 6.3 | 4.2 | 3.2 |
| Percent error in $T_w^*$ | | | | |
| 1200 | 14.1 | 9.7 | 6.5 | 4.4 |
| 2000 | 20.0 | 9.8 | 5.7 | 3.8 |
| Transmittance at 3500 $cm^{-1}$ | | | | |
| 1200 | 0.703 | 0.591 | 0.465 | 0.333 |
| 2000 | .713 | .602 | .476 | .343 |

## TABLE IV. - PARAMETER INDEX CONTROL

| KEY | KEY1(KEY) | KEY2(KEY) | KEY3(KEY) | Variable parameters | |
|---|---|---|---|---|---|
| | K1 | K2 | K3 | Fig. 1(a), PROF=1 | Fig. 1(b), PROF=2 |
| 1 | 1 | 3 | 1 | $n_T$ $T_c$ $p_c$ | $T_c$ $p_c$ $T_w^*$ |
| 2 | 1 | 2 | 1 | $n_T$ $T_c$ | $T_c$ $p_c$ |
| 3 | 1 | 3 | 2 | $n_T$ $p_c$ | $T_c$ $T_w^*$ |
| 4 | 1 | 1 | 1 | $n_T$ | $T_c$ |
| 5 | 2 | 3 | 1 | $T_c$ $p_c$ | $p_c$ $T_w^*$ |
| 6 | 2 | 2 | 1 | $T_c$ | $p_c$ |
| 7 | 3 | 3 | 1 | $p_c$ | $T_w^*$ |
| 8 | 0 | 0 | 0 | None | None |




(a) Non-isothermal temperature profiles, $T_w$ = constant.

(b) Near-isothermal temperature profiles, with $T_w$ = constant and boundary layer thickness $x_1$ = constant.

(c) Partial pressure profile for each absorbing gas.

Figure 1. - Assumed profile functions.

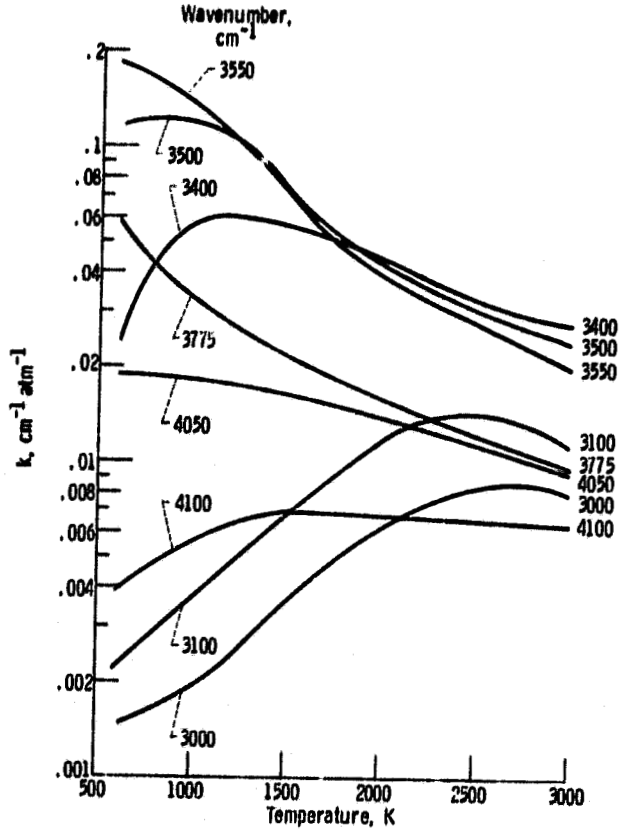



Figure 2. - Absorption coefficient for $H_2O$.

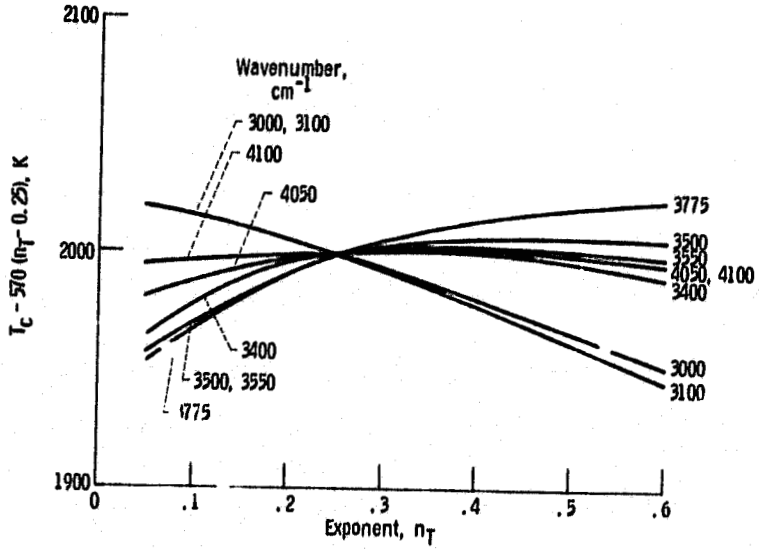



Figure 3. - Test of wavenumbers for profile of figure 1(a) with $T_w$ = 1000 K, $p_c$ = 0.35 atm, $p_w$ = 0.30 atm, $n_p$ = 0.50, path length 100 cm Hydrogen-air combustion at 1 atm.

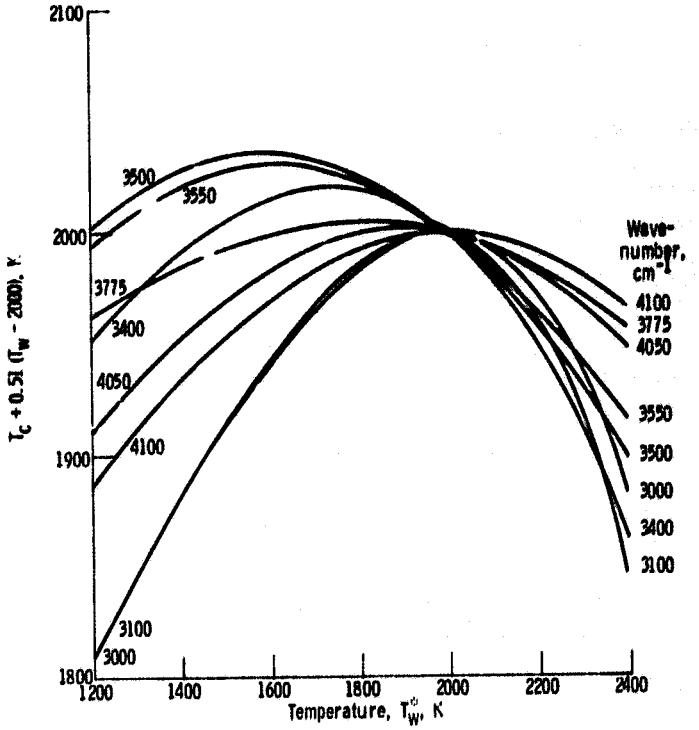
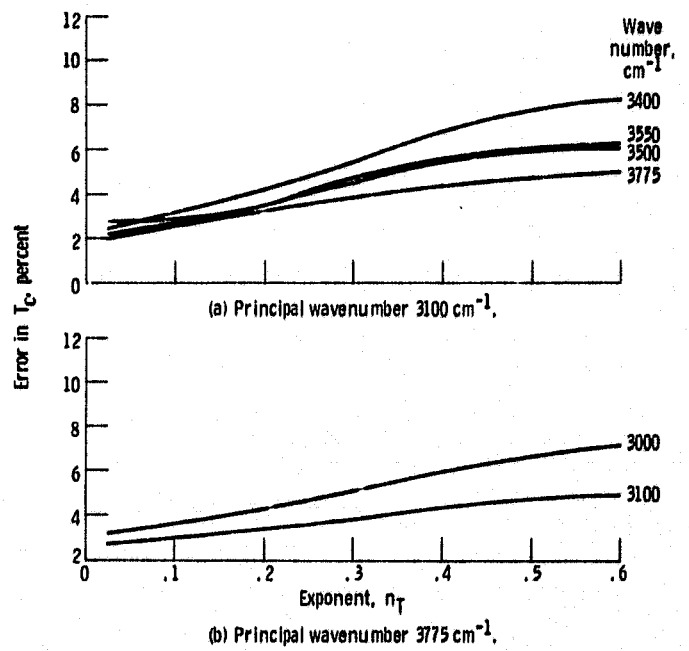



Figure 4. - Test of wavenumbers for profile of figure 1(b) with $n_T$ = 0.5, $p_c$ = 0.35 atm, $p_w$ = 0.30 atm, $n_D$ = 0.50, path length 100 cm. Hydrogen-air combustion at 1 atm.




(a) Principal wavenumber 3100 cm$^{-1}$.

(b) Principal wavenumber 3775 cm$^{-1}$.

Figure 5. - Estimated error in $T_c$ due solely to errors in radiometer and tabulated absorption coefficients. Profile of figure 1(a), with $T_c$ = 2000 K, $T_w$ = 1000 K, $p_c$ = 0.35 atm, $p_w$ = 0.65 atm, $n_D$ = 0.50, path length 100 cm. Hydrogen-air combustion at 1 atm. Error of radiometry 1 percent, error of tabulated absorption coefficient 5 percent.

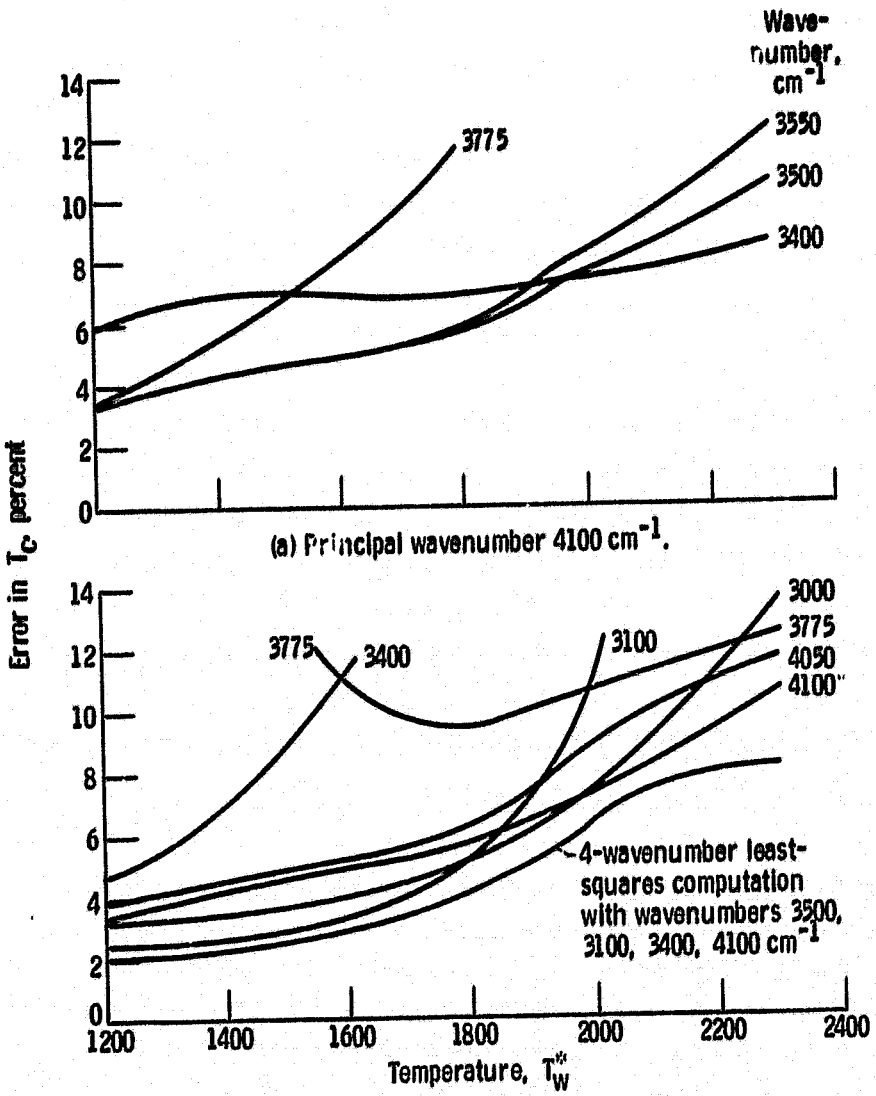



Figure 6. - Estimated error in $T_c$ due solely to errors in radiometry and in tabulated absorption coefficients. Profile of figure 1(b) with $T_c$ = 2000 K, $n_T$ = 0.5, $p_c$ = 0.35 atm, $p_w$ = 0.30 atm, $n_p$ = 0.50, path length 100 cm. Hydrogen-air combustion at 1 atm. Error of radiometry 1 percent, tabulated absorption coefficient 5 percent.

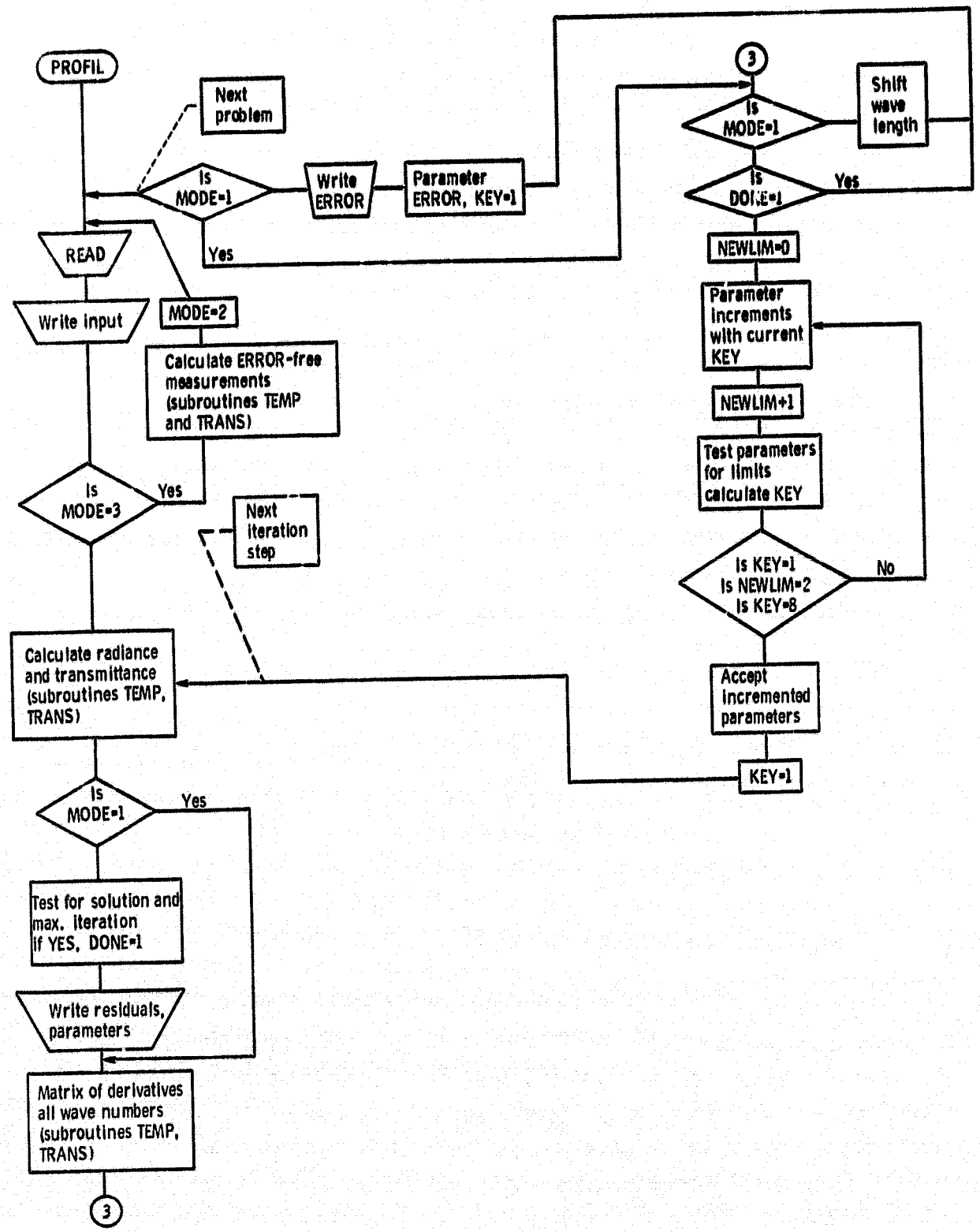



Figure 7. - Flow chart for PROFIL.

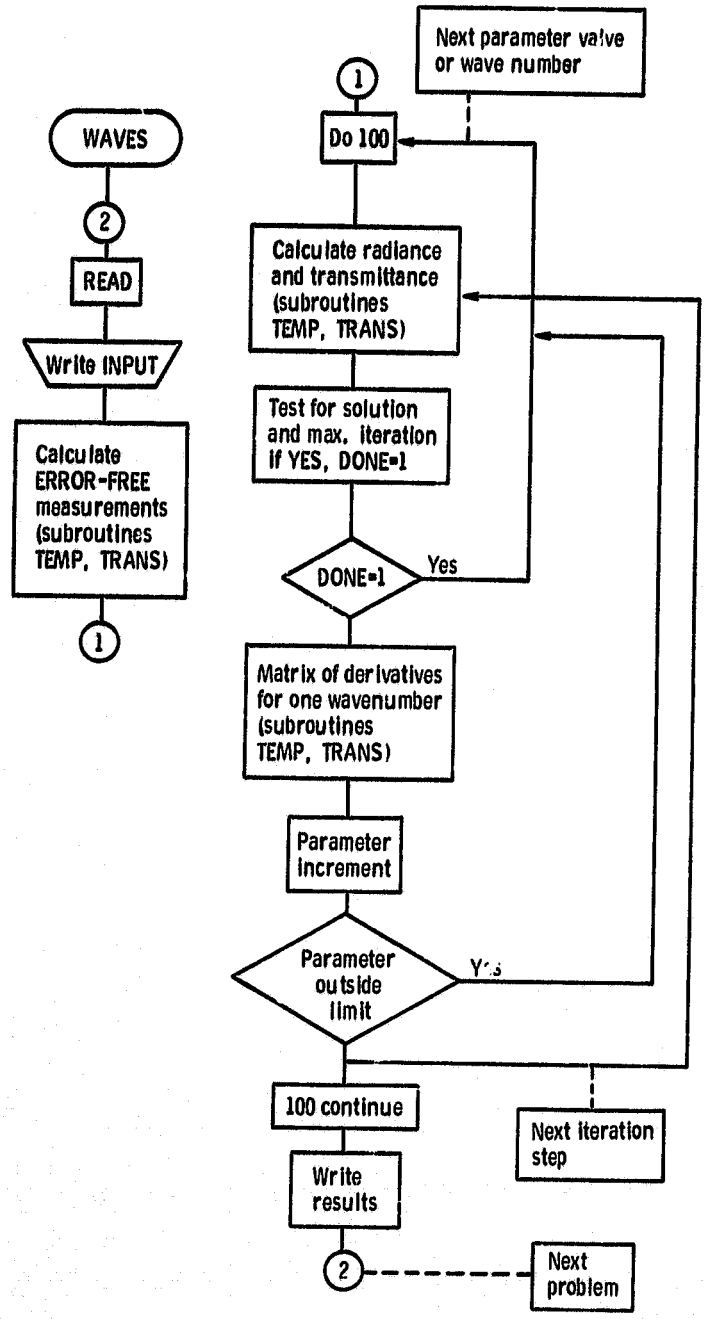
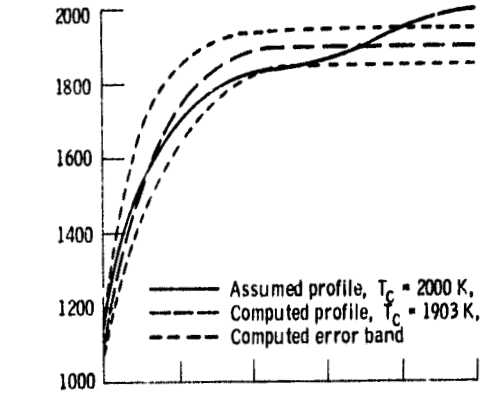
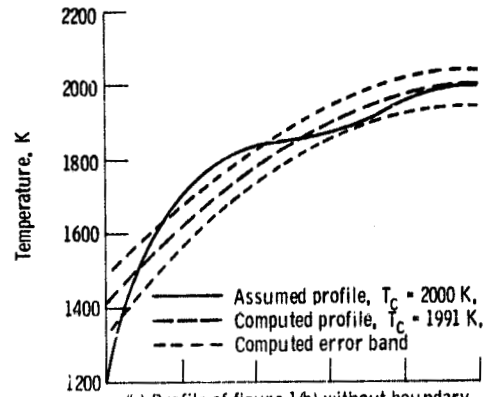


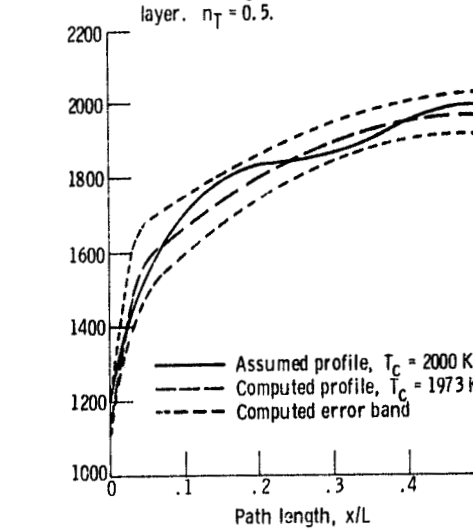

Figure 8. - Flow chart for WAVES.




(a) Profile of figure 1(a) with $T_w$ = 1100 K.




(b) Profile of figure 1(b) without boundary layer. $n_T$ = 0.5.




(c) Profile of figure 1(b) with boundary layer. $n_T$ = 0.5, $T_w$ = 1100 K.

Figure 9. - Example of profile with high-temperature core. Wavenumbers of measurement 3500 and 3100 $cm^{-1}$.